



STIC Search Report

Biotech-Chem Library

STIC Database Tracking Number: 120882

TO: Edward Ward
Location: 3d14/3d11
Art Unit: 1654
Friday, May 07, 2004
Case Serial Number: 10/612885

3D11

From: Paul Schulwitz
Location: Biotech-Chem Library
REM-1A65
Phone: (571)272-2527

paul.schulwitz@uspto.gov

Search Notes

Examiner Ward,

See attached results.

If you have any questions about this search feel free to contact me at any time.

Thank you for using STIC search services!

Paul Schulwitz
Technical Information Specialist
STIC Biotech/Chem Library
(571)272-2527



05P 6/5

Access DB# 120882

SEARCH REQUEST FORM

Scientific and Technical Information Center

Requester's Full Name: Edward Ward Examiner #: 67950 Date: May 2, 2004
Art Unit: 1834 Phone Number: 471-277-0886 Serial Number: 1W6288
Mail Box and Bldg/Room Location: Room 3011 / Room 3014 Results Format Preferred (circle): PAPER DISK E-MAIL

If more than one search is submitted, please prioritize searches in order of need.

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc. if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

Title of Invention: _____

Inventors (please provide full names): Oleson, Lennart

Earliest Priority Filing Date: _____

For Sequence Searches Only Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.

1- AA-23 me Sequence #1 and the compound

RECEIVED
MAY - 3 2004
STIC/STIC

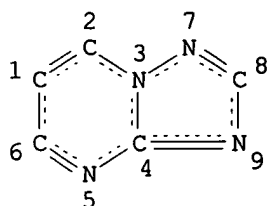
Structures and seq id #1

Ward 10/612,885

May 7, 2004

=> d que 134

L13 STR



NODE ATTRIBUTES:

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DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

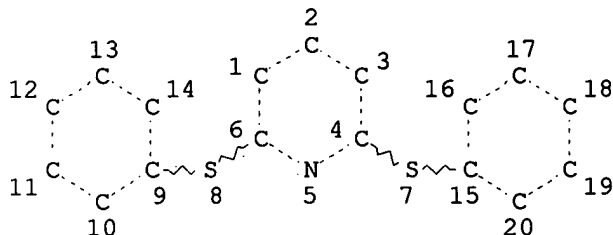
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NUMBER OF NODES IS 9

STEREO ATTRIBUTES: NONE

L15 11751 SEA FILE=REGISTRY SSS FUL L13

L16 STR



NODE ATTRIBUTES:

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DEFAULT ECLEVEL IS LIMITED

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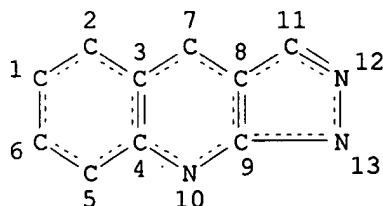
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L18 STR



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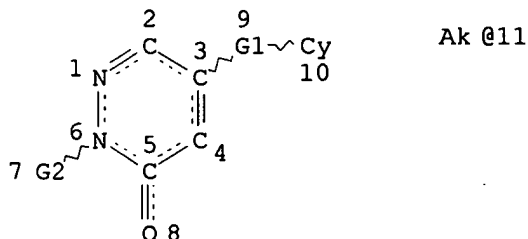
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RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 13

STEREO ATTRIBUTES: NONE

L19 1779 SEA FILE=REGISTRY SSS FUL L18
L20 STR



VAR G1=O/S

VAR G2=H/11

NODE ATTRIBUTES:

CONNECT IS E1 RC AT 11
DEFAULT MLEVEL IS ATOM
GGCAT IS UNS AT 10
GGCAT IS LOC AT 11
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 11

STEREO ATTRIBUTES: NONE

L21 158 SEA FILE=REGISTRY SSS FUL L20
L33 33 SEA FILE=REGISTRY ABB=ON PLU=ON ~~(OR FILE=REGISTRY SSS FUL L20)~~ *SID #1*

~~L34~~ *134* SEA FILE=HCAPLUS ABB=ON PLU=ON L33 AND (L15 OR L17 OR L19 OR L21)

=> d ibib abs 134

L34 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2004:41501 HCAPLUS

DOCUMENT NUMBER: 140:87744

TITLE: Affinity small molecules for the EPO receptor

INVENTOR(S): Olsson, Lennart; Naranda, Tatjana

PATENT ASSIGNEE(S): Receptron, Inc., USA

SOURCE: PCT Int. Appl., 85 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004005323	A2	20040115	WO 2003-US21394	20030703

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
PL, PT, RO, RU, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA,
UG, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG,
CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC,
NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ,
GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 2002-393360P P 20020703
US 2002-393361P P 20020703
US 2002-394110P P 20020703

OTHER SOURCE(S): MARPAT 140:87744

AB Compds. are provided that complex with the modulating domain of erythropoietin receptor (EPO-R) for use with EPO-R to determine the presence of EPO-R, the ability of other mols. to bind to the modulating domain in competitive assays and to induce a signal by EPO-R into a cell when bound by the subject compds. in a physiol. environment. The compds. are characterized by having a six-membered heterocyclic ring comprising at least one nitrogen atom and include substituted triazolopyrimidine, pyridazinone, pyridine and piperidine.

L36 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2004 ACS on STN

RN 239133-03-0 REGISTRY

CN L-Tyrosine, L-glutamyl-L-arginyl-L-valyl-L- α -glutamyl-L-isoleucyl-L-leucyl-L- α -glutamylglycyl-L-arginyl-L-threonyl-L- α -glutamyl-L-cysteinyl-L-valyl-L-leucyl-L-seryl-L-asparaginyl-L-leucyl-L-arginylglycyl-L-arginyl-L-threonyl-L-arginyl- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN 11: PN: US6333031 SEQID: 11 claimed protein

CN 1: PN: WO2004005323 SEQID: 1 unclaimed sequence

CN 30: PN: WO03020746 SEQID: 30 unclaimed sequence

CN 30: PN: WO2004020588 SEQID: 30 unclaimed sequence

FS PROTEIN SEQUENCE; STEREOSEARCH

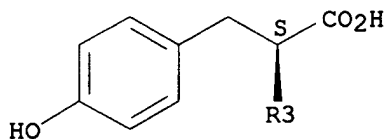
MF C115 H198 N40 O36 S

SR CA

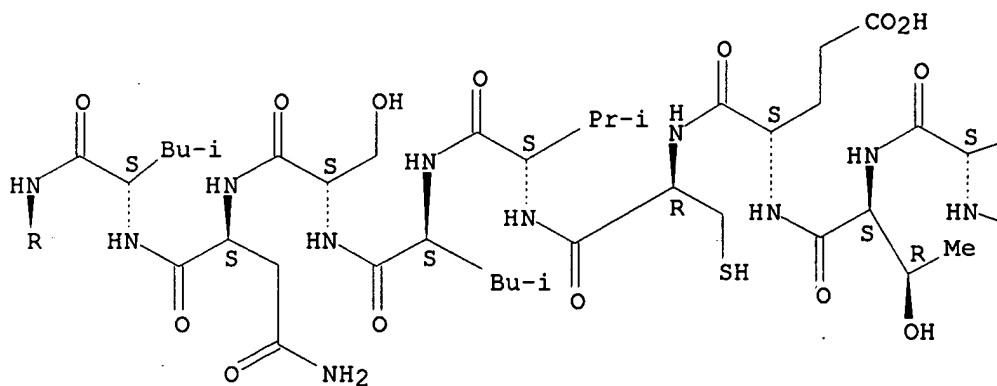
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Absolute stereochemistry.

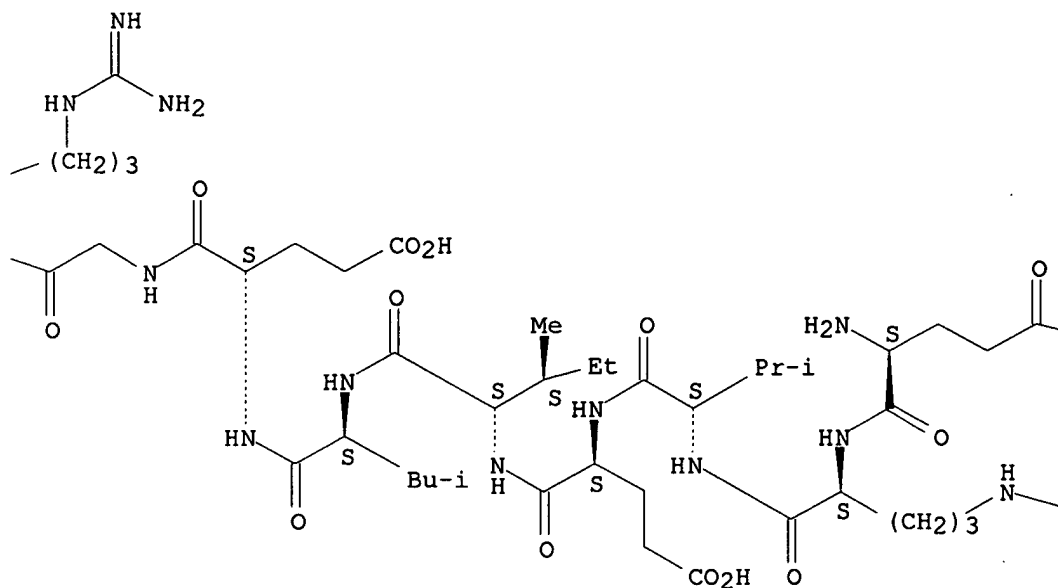
PAGE 1-A



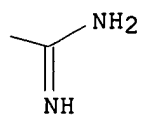
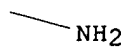
PAGE 2-A



PAGE 2-B



PAGE 2-C



The chemical structure is a complex molecule, likely a peptide derivative, featuring several functional groups and labeled components. It includes amide bonds, a hydroxyl group (OH), a methyl group (Me), and a guanidino group (NH-C(=NH)-NH2). The structure is labeled with R, R2, Me, and (CH2)3, indicating specific substituents and side chains. The molecule is shown in a perspective view, with bonds indicating stereochemistry.

NC(=N)NC(C)C(=O)N[R3]

Searched by Paul Schulwitz (571)272-2527

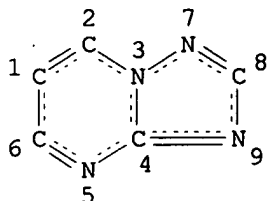
Structures + Text

Ward 10/612,885

May 7, 2004

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L10 1 SEA FILE=REGISTRY ABB=ON PLU=ON 11096-26-7
 L11 1095 SEA FILE=HCAPLUS ABB=ON PLU=ON ERYTHROPOIETIN RECEPTORS+OLD/C
 T
 L13 STR

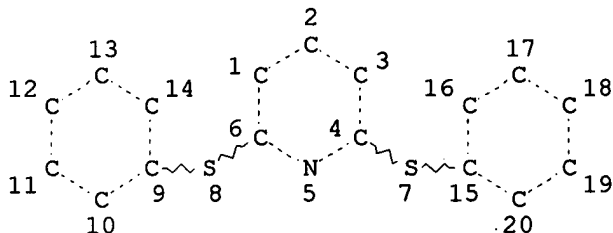


(1)

NODE ATTRIBUTES:
 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
 RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 9

STEREO ATTRIBUTES: NONE
 L15 11751 SEA FILE=REGISTRY SSS FUL L13
 L16 STR

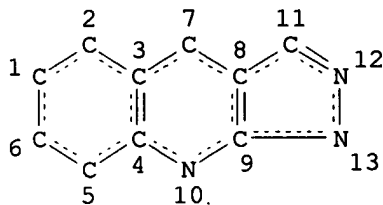


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NODE ATTRIBUTES:
 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
 RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 20

STEREO ATTRIBUTES: NONE
 L17 65 SEA FILE=REGISTRY SSS FUL L16
 L18 STR



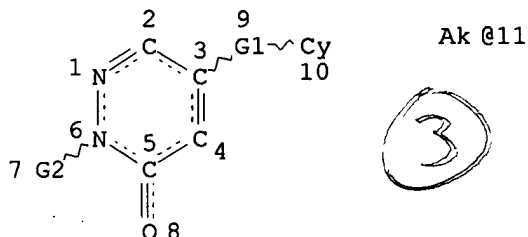
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NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 13

STEREO ATTRIBUTES: NONE
L19 1779 SEA FILE=REGISTRY SSS FUL L18
L20 STR



VAR G1=O/S
VAR G2=H/11
NODE ATTRIBUTES:
CONNECT IS E1 RC AT 11
DEFAULT MLEVEL IS ATOM
GGCAT IS UNS AT 10
GGCAT IS LOC AT 11
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 11

STEREO ATTRIBUTES: NONE
L21 158 SEA FILE=REGISTRY SSS FUL L20
L22 2621 SEA FILE=HCAPLUS ABB=ON PLU=ON L15 OR L17 OR L19 OR L21
~~L24 1 SEA FILE=HCAPLUS ABB=ON PLU=ON (L11 OR L10 OR EPO OR~~
ERYTHROPO?) AND L22

~~=> (L24, HCAPLUS, ABB=ON, PLU=ON, HITING, HATSTR)~~

L24 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2004:41501 HCAPLUS
DOCUMENT NUMBER: 140:87744
TITLE: Affinity small molecules for the EPO receptor
INVENTOR(S): Olsson, Lennart; Naranda, Tatjana
PATENT ASSIGNEE(S): Receptron, Inc., USA
SOURCE: PCT Int. Appl., 85 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004005323	A2	20040115	WO 2003-US21394	20030703
<p>W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM</p> <p>RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG</p>				
PRIORITY APPLN. INFO.:			US 2002-393360P	P 20020703
			US 2002-393361P	P 20020703
			US 2002-394110P	P 20020703
OTHER SOURCE(S): MARPAT 140:87744				
AB	Compds. are provided that complex with the modulating domain of erythropoietin receptor (EPO-R) for use with EPO -R to determine the presence of EPO-R , the ability of other mols. to bind to the modulating domain in competitive assays and to induce a signal by EPO-R into a cell when bound by the subject compds. in a physiol. environment. The compds. are characterized by having a six-membered heterocyclic ring comprising at least one nitrogen atom and include substituted triazolopyrimidine, pyridazinone, pyridine and piperidine.			
IC	ICM C07K			
CC	1-12 (Pharmacology)			
ST	Section cross-reference(s): 2			
IT	EPO receptor modulator small mol			
IT	Proteins			
	RL: BSU (Biological study, unclassified); BIOL (Biological study) (Bcl-xL, expression; affinity small mols. for erythropoietin (EPO) receptor and EPO receptor modulating sequence in relation to modulating the response to the stimulus of hematopoietic or neuronal cells and treatment of anemia)			
IT	Peptides, biological studies			
	RL: BSU (Biological study, unclassified); BUU (Biological use, unclassified); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (EPO receptor modulating sequence; affinity small mols. for erythropoietin (EPO) receptor and EPO receptor modulating sequence in relation to modulating the response to the stimulus of hematopoietic or neuronal cells and treatment of anemia)			
IT	Cell membrane			
	(EPO receptors of; affinity small mols. for erythropoietin (EPO) receptor and EPO receptor modulating sequence in relation to modulating the response to the stimulus of hematopoietic or neuronal cells and treatment of anemia)			
IT	Anemia (disease)			
	Cell proliferation			
	Combinatorial library			
	Drug delivery systems			
	Drug screening			
	Erythrocyte			

Erythropoiesis

Hematocrit

Hematopoietic precursor cell

Human

Reticulocyte

(affinity small mols. for **erythropoietin (EPO)**
receptor and **EPO** receptor modulating sequence in relation to
modulating the response to the stimulus of hematopoietic or neuronal
cells and treatment of anemia)

IT **Erythropoietin receptors**

RL: BSU (Biological study, unclassified); BUU (Biological use,
unclassified); BIOL (Biological study); USES (Uses)

(affinity small mols. for **erythropoietin (EPO)**
receptor and **EPO** receptor modulating sequence in relation to
modulating the response to the stimulus of hematopoietic or neuronal
cells and treatment of anemia)

IT Nerve

(neuron; affinity small mols. for **erythropoietin (EPO)**
) receptor and **EPO** receptor modulating sequence in relation
to modulating the response to the stimulus of hematopoietic or neuronal
cells and treatment of anemia)

IT Cytoprotective agents

(neuroprotective; affinity small mols. for **erythropoietin (EPO)**
EPO receptor and **EPO** receptor modulating sequence in
relation to modulating the response to the stimulus of hematopoietic or
neuronal cells and treatment of anemia)

IT 2503-56-2 40775-78-8 51646-16-3

51646-17-4 51646-19-6 51646-43-6

56347-20-7 63901-48-4 90559-98-1

90815-61-5 113967-71-8 113967-74-1

194342-06-8 212074-47-0 244167-89-3

245082-87-5 245413-82-5 259683-29-9

261704-08-9 261704-09-0 262291-81-6

263267-38-5 287728-46-5 303145-64-4

303145-73-5 338793-16-1 645337-19-5

645337-20-8 645337-21-9 645337-22-0

645337-23-1 645337-24-2 645337-25-3

RL: BSU (Biological study, unclassified); BUU (Biological use,
unclassified); PAC (Pharmacological activity); THU (Therapeutic use); BIOL
(Biological study); USES (Uses)

(affinity small mols. for **erythropoietin (EPO)**
receptor and **EPO** receptor modulating sequence in relation to
modulating the response to the stimulus of hematopoietic or neuronal
cells and treatment of anemia)

IT 11096-26-7, **Erythropoietin**

RL: BSU (Biological study, unclassified); PAC (Pharmacological activity);
THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(affinity small mols. for **erythropoietin (EPO)**
receptor and **EPO** receptor modulating sequence in relation to
modulating the response to the stimulus of hematopoietic or neuronal
cells and treatment of anemia)

IT 239133-03-0 645415-22-1

RL: PRP (Properties)

(unclaimed sequence; affinity small mols. for the **EPO**
receptor)

IT 2503-56-2 40775-78-8 51646-16-3

51646-17-4 51646-19-6 51646-43-6

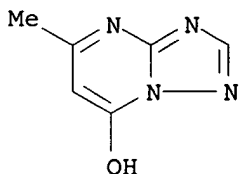
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 194342-06-8 212074-47-0 244167-89-3
 245082-87-5 245413-82-5 259683-29-9
 261704-08-9 261704-09-0 262291-81-6
 263267-38-5 287728-46-5 303145-64-4
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 645337-20-8 645337-21-9 645337-22-0
 645337-23-1 645337-24-2 645337-25-3

RL: BSU (Biological study, unclassified); BUU (Biological use, unclassified); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(affinity small mols. for **erythropoietin (EPO)** receptor and **EPO** receptor modulating sequence in relation to modulating the response to the stimulus of hematopoietic or neuronal cells and treatment of anemia)

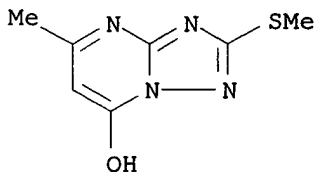
RN 2503-56-2 HCAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidin-7-ol, 5-methyl- (9CI) (CA INDEX NAME)



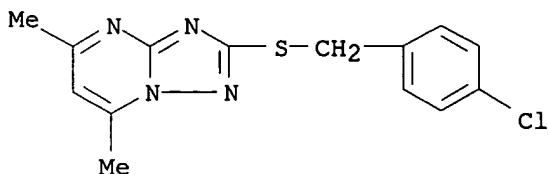
RN 40775-78-8 HCAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidin-7-ol, 5-methyl-2-(methylthio)- (9CI) (CA INDEX NAME)



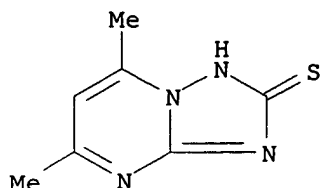
RN 51646-16-3 HCAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidine, 2-[[(4-chlorophenyl)methyl]thio]-5,7-dimethyl- (9CI) (CA INDEX NAME)



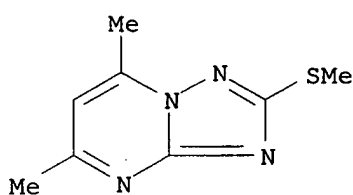
RN 51646-17-4 HCAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidine-2(1H)-thione, 5,7-dimethyl- (9CI) (CA INDEX NAME)



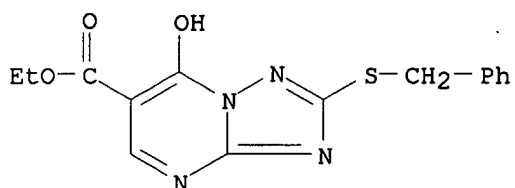
RN 51646-19-6 HCAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidine, 5,7-dimethyl-2-(methylthio)- (9CI) (CA INDEX NAME)



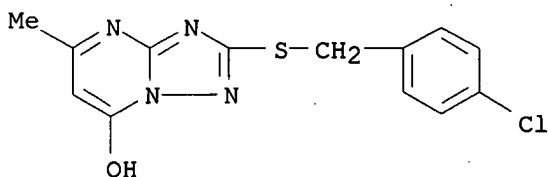
RN 51646-43-6 HCAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidine-6-carboxylic acid, 7-hydroxy-2-[(phenylmethyl)thio]-, ethyl ester (9CI) (CA INDEX NAME)



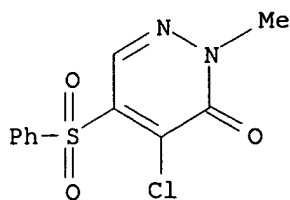
RN 56347-20-7 HCAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidin-7-ol, 2-[[4-(4-chlorophenyl)methyl]thio]-5-methyl- (9CI) (CA INDEX NAME)



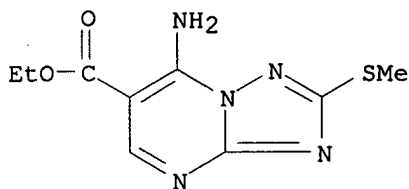
RN 63901-48-4 HCAPLUS

CN 3(2H)-Pyridazinone, 4-chloro-2-methyl-5-(phenylsulfonyl)- (9CI) (CA INDEX NAME)



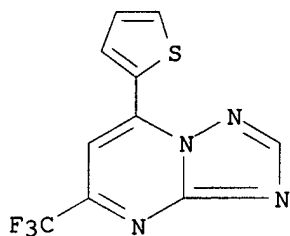
RN 90559-98-1 HCAPLUS

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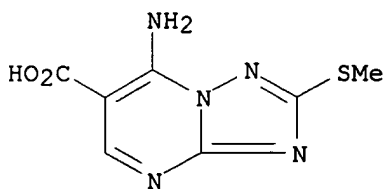
RN 90815-61-5 HCAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidine, 7-(2-thienyl)-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)



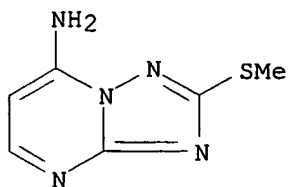
RN 113967-71-8 HCAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidine-6-carboxylic acid, 7-amino-2-(methylthio)- (9CI) (CA INDEX NAME)



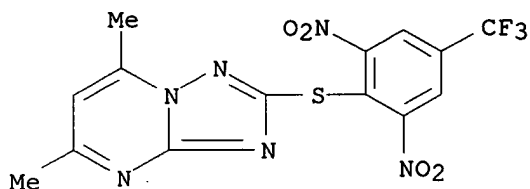
RN 113967-74-1 HCAPLUS

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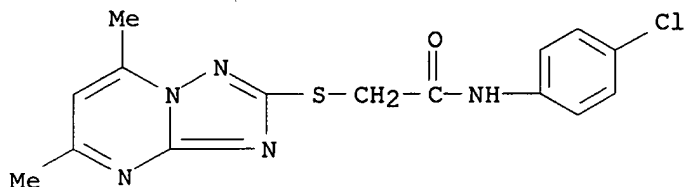
RN 194342-06-8 HCAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidine, 2-[[2,6-dinitro-4-(trifluoromethyl)phenyl]thio]-5,7-dimethyl- (9CI) (CA INDEX NAME)



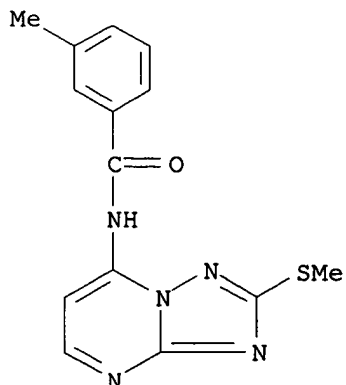
RN 212074-47-0 HCAPLUS

CN Acetamide, N-(4-chlorophenyl)-2-[(5,7-dimethyl[1,2,4]triazolo[1,5-a]pyrimidin-2-yl)thio]- (9CI) (CA INDEX NAME)

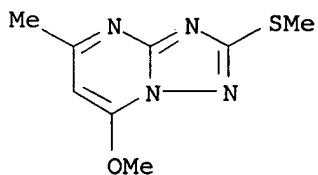


RN 244167-89-3 HCAPLUS

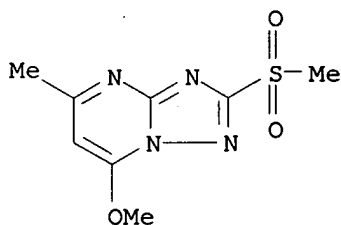
CN Benzamide, 3-methyl-N-[2-(methylthio)[1,2,4]triazolo[1,5-a]pyrimidin-7-yl]- (9CI) (CA INDEX NAME)



RN 245082-87-5 HCAPLUS

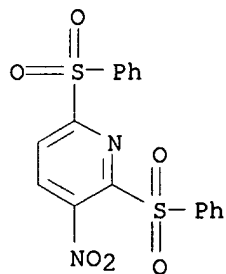
CN [1,2,4]Triazolo[1,5-a]pyrimidine, 7-methoxy-5-methyl-2-(methylthio)- (9CI)
(CA INDEX NAME)

RN 245413-82-5 HCAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidine, 7-methoxy-5-methyl-2-(methylsulfonyl)-
(9CI) (CA INDEX NAME)

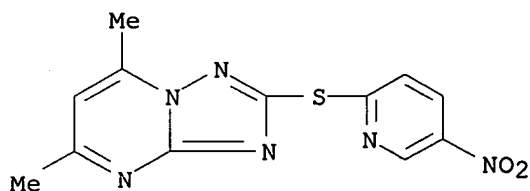
RN 259683-29-9 HCAPLUS

CN Pyridine, 3-nitro-2,6-bis(phenylsulfonyl)- (9CI) (CA INDEX NAME)



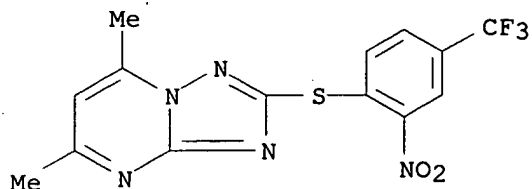
RN 261704-08-9 HCAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidine, 5,7-dimethyl-2-[(5-nitro-2-pyridinyl)thio]- (9CI) (CA INDEX NAME)



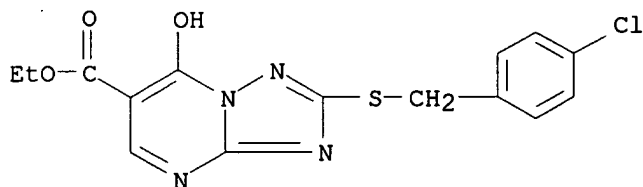
RN 261704-09-0 HCAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidine, 5,7-dimethyl-2-[[2-nitro-4-(trifluoromethyl)phenyl]thio]- (9CI) (CA INDEX NAME)



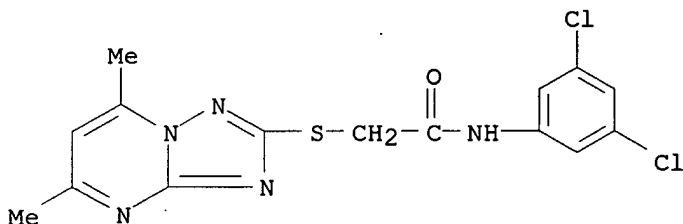
RN 262291-81-6 HCAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidine-6-carboxylic acid, 2-[[[4-chlorophenyl)methyl]thio]-7-hydroxy-, ethyl ester (9CI) (CA INDEX NAME)



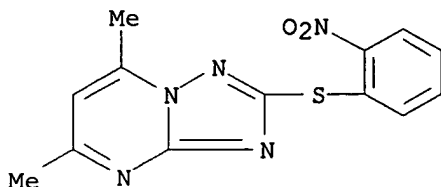
RN 263267-38-5 HCAPLUS

CN Acetamide, N-(3,5-dichlorophenyl)-2-[(5,7-dimethyl[1,2,4]triazolo[1,5-a]pyrimidin-2-yl)thio]- (9CI) (CA INDEX NAME)

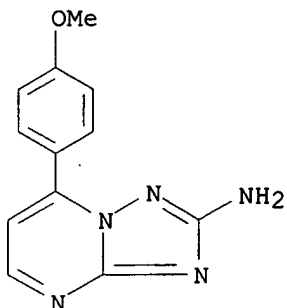


RN 287728-46-5 HCAPLUS

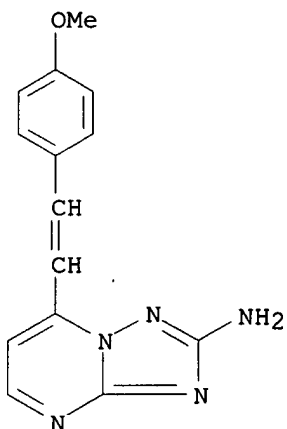
CN [1,2,4]Triazolo[1,5-a]pyrimidine, 5,7-dimethyl-2-[(2-nitrophenyl)thio]- (9CI) (CA INDEX NAME)



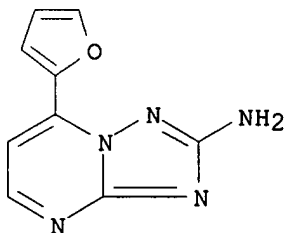
RN 303145-64-4 HCAPLUS
CN [1,2,4]Triazolo[1,5-a]pyrimidin-2-amine, 7-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



RN 303145-73-5 HCAPLUS
CN [1,2,4]Triazolo[1,5-a]pyrimidin-2-amine, 7-[2-(4-methoxyphenyl)ethenyl]- (9CI) (CA INDEX NAME)

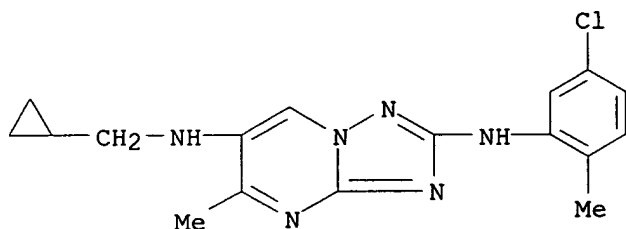


RN 338793-16-1 HCAPLUS
CN [1,2,4]Triazolo[1,5-a]pyrimidin-2-amine, 7-(2-furanyl)- (9CI) (CA INDEX NAME)



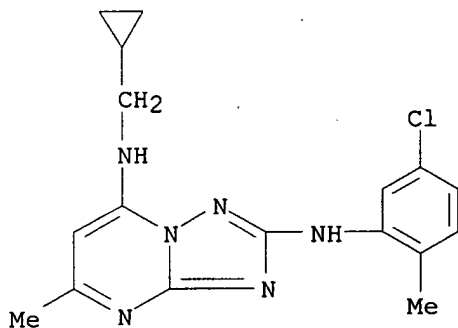
RN 645337-19-5 HCAPLUS
CN [1,2,4]Triazolo[1,5-a]pyrimidine-2,6-diamine, N2-(5-chloro-2-methylphenyl)-

N6-(cyclopropylmethyl)-5-methyl- (9CI) (CA INDEX NAME)



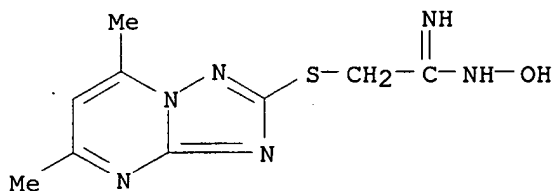
RN 645337-20-8 HCAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidine-2,7-diamine, N2-(5-chloro-2-methylphenyl)-
N7-(cyclopropylmethyl)-5-methyl- (9CI) (CA INDEX NAME)



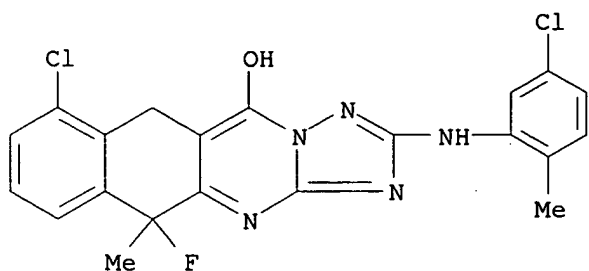
RN 645337-21-9 HCAPLUS

CN Ethanimidamide, 2-[(5,7-dimethyl[1,2,4]triazolo[1,5-a]pyrimidin-2-yl)thio]-
N-hydroxy- (9CI) (CA INDEX NAME)



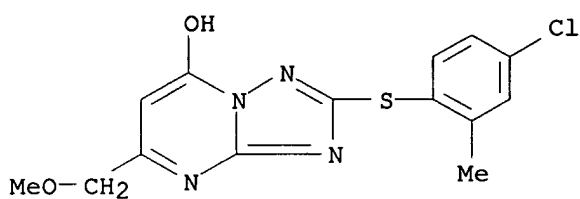
RN 645337-22-0 HCAPLUS

CN Benzo[g][1,2,4]triazolo[5,1-b]quinazolin-11-ol, 9-chloro-2-[(5-chloro-2-methylphenyl)amino]-5-fluoro-5,10-dihydro-5-methyl- (9CI) (CA INDEX NAME)



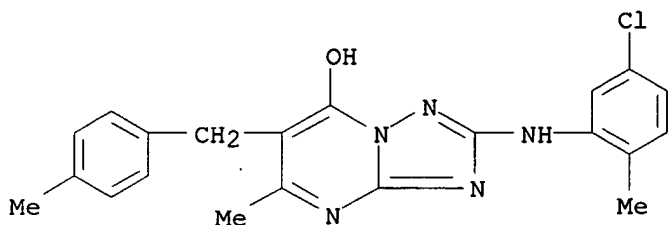
RN 645337-23-1 HCAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidin-7-ol, 2-[(4-chloro-2-methylphenyl)thio]-5-(methoxymethyl)- (9CI) (CA INDEX NAME)



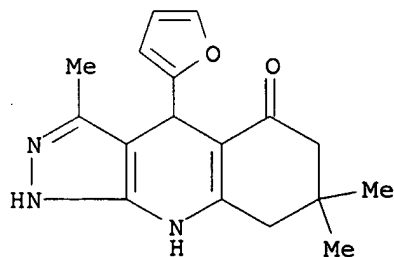
RN 645337-24-2 HCAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidin-7-ol, 2-[(5-chloro-2-methylphenyl)amino]-5-methyl-6-[(4-methylphenyl)methyl]- (9CI) (CA INDEX NAME)



RN 645337-25-3 HCAPLUS

CN 5H-Pyrazolo[3,4-b]quinolin-5-one, 4-(2-furanyl)-1,4,6,7,8,9-hexahydro-3,7,7-trimethyl- (9CI) (CA INDEX NAME)



IT 11096-26-7, Erythropoietin

RL: BSU (Biological study, unclassified); PAC (Pharmacological activity);
THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(affinity small mols. for **erythropoietin (EPO)**
receptor and **EPO** receptor modulating sequence in relation to
modulating the response to the stimulus of hematopoietic or neuronal
cells and treatment of anemia)

RN 11096-26-7 HCAPLUS

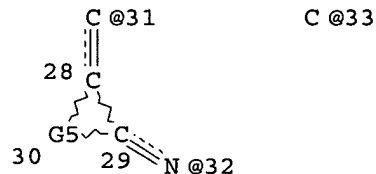
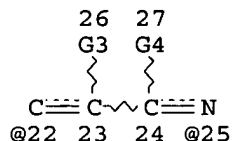
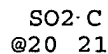
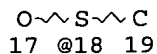
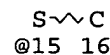
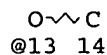
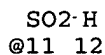
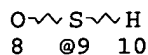
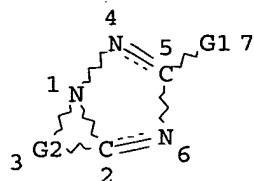
CN Erythropoietin (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

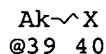
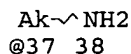
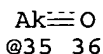
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L9

STR



Ak @34



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VAR G3=H/33

VAR G4=H/34/35/37/39

REP G5=(1-20) A

NODE ATTRIBUTES:

NSPEC IS RC AT 14

NSPEC IS RC AT 16

NSPEC IS RC AT 19

NSPEC IS RC AT 21

NSPEC IS RC AT 33

CONNECT IS E1 RC AT 8

CONNECT IS E2 RC AT 9

CONNECT IS E2 RC AT 15

CONNECT IS E1 RC AT 17

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CONNECT IS E1 RC AT 34

DEFAULT MLEVEL IS ATOM

GGCAT IS LOC AT 34

GGCAT IS LOC AT 35

GGCAT IS LOC AT 37

GGCAT IS LOC AT 39

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 40

STEREO ATTRIBUTES: NONE

L11 3288 SEA FILE=REGISTRY SSS FUL L9

L18 678 SEA FILE=HCAPLUS ABB=ON PLU=ON L11(L)BIOL/RL

L19 9 SEA FILE=HCAPLUS ABB=ON PLU=ON L11(L)MODULAT?

L20 9 SEA FILE=HCAPLUS ABB=ON PLU=ON L18 AND L19

L23 4 SEA FILE=HCAPLUS ABB=ON PLU=ON L18 AND (NEURON? OR HEMATOPOI?
OR ANEMI?)
L24 12 SEA FILE=HCAPLUS ABB=ON PLU=ON L23 OR L20

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L24 ANSWER 1 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2004:80683 HCAPLUS

DOCUMENT NUMBER: 140:128433

TITLE: Preparation of piperazinyl-2(1H)-pyrazinones for
treatment of 5-HT_{2A} receptor-related disorders

INVENTOR(S): Nilsson, Bjoern; Thor, Markus; Cernerud, Magnus;
Lundstroem, Helena

PATENT ASSIGNEE(S): Biovitrum Ab, Swed.

SOURCE: PCT Int. Appl., 90 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

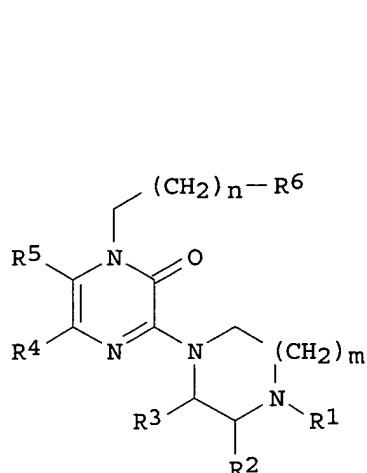
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004009586	A1	20040129	WO 2003-SE1102	20030625
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RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			

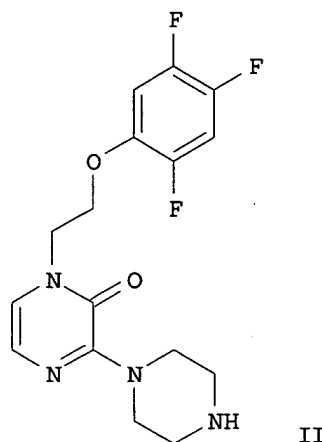
PRIORITY APPLN. INFO.: SE 2002-2287 A 20020719
US 2002-426240P P 20021114

OTHER SOURCE(S): MARPAT 140:128433

GI



I



II

AB Title compds. I [wherein $m = 1-2$; $n = 0-4$; $R_1 = H$, (methoxy)alkyl, 2-hydroxyethyl, alkoxycarbonyl, or (un)substituted (hetero)arylalkyl or (hetero)aryloxyalkyl; R_2 and $R_3 =$ independently H or Me ; R_4 and $R_5 =$ independently H , halo, or Me ; or R_4 and R_5 together with the ring to which the C atoms are attached = a 1H-quinoxalin-2-one nucleus; $R_6 =$ (un)substituted (hetero)aryloxy, (hetero)arylthio, (hetero)arylamino, (hetero)aryl, or (hetero)arylcabonyl; with provisos; and pharmaceutically acceptable salts, hydrates, geometrical isomers, tautomers, optical isomers, N-oxides, or prodrugs thereof] were prepared as 5-HT_{2A} receptor modulators. For example, condensation of 2,4,5-trifluorophenol with 2-[3-(4-tert-butoxycarbonyl-1-piperazinyl)pyrazinyl]ethanol in the presence of TMAD and polymer-bound PPh_3 in CH_2Cl_2 , followed by deprotection with TFA/ CH_2Cl_2 / H_2O and salt formation gave II•HCl (85%). The latter displaced 3H-labeled LSD bound to membranes, prepared from transfected CHO cell line stably expressing the human 5-HT_{2A} receptor protein, with a receptor affinity value of $K_i = 2.2$ nM. Thus, I and their pharmaceutical compns. are useful for the treatment of 5-HT_{2A} receptor-related disorders, such as Raynaud's phenomenon, hypertension, fibromyalgia, thrombotic disorders, Alzheimer's disease, depression, COPD, glaucoma, eating disorders, etc. (no data).

IC. ICM C07D239-02

ICS C07D295-033; A61K031-496; A61P003-04; A61P003-10; A61P009-00; A61P015-00; A61P025-28; A61P025-24

CC 28-17 (Heterocyclic Compounds (More Than One Hetero Atom))

Section cross-reference(s): 1, 63

IT 651046-48-9P 651046-50-3P, 1-[2-[(2-Oxo-2H-chromen-7-yl)oxy]ethyl]-3-(1-piperazinyl)-1H-pyrazin-2-one hydrochloride 651046-52-5P, 3-(1-Piperazinyl)-1-[2-(2,4,5-trifluorophenoxy)ethyl]-1H-pyrazin-2-one hydrochloride 651046-53-6P, 3-(1-Piperazinyl)-1-[2-(2,3,5,6-tetrafluorophenoxy)ethyl]-1H-pyrazin-2-one hydrochloride 651046-54-7P, 1-[2-(2,3,4,5,6-Pentafluorophenoxy)ethyl]-3-(1-piperazinyl)-1H-pyrazin-2-one hydrochloride 651046-55-8P, 1-[2-(4-Chloro-2-fluorophenoxy)ethyl]-3-(1-piperazinyl)-1H-pyrazin-2-one 651046-56-9P, 1-[2-(3-Cyanophenoxy)ethyl]-3-(1-piperazinyl)-1H-pyrazin-2-one 651046-57-0P, 1-[2-(4-Cyclopentylphenoxy)ethyl]-3-(1-piperazinyl)-1H-pyrazin-2-one 651046-58-1P, 1-[2-[(1,2-Benzisoxazol-3-yl)oxy]ethyl]-3-(1-piperazinyl)-1H-pyrazin-2-one dihydrochloride 651046-59-2P, 1-[2-(3-Methoxyphenoxy)ethyl]-3-(1-piperazinyl)-1H-pyrazin-2-one 651046-60-5P, 1-[2-[3-(Butyloxy)phenoxy]ethyl]-3-(1-piperazinyl)-1H-pyrazin-2-one

651046-61-6P, 1-[2-[[[1,1'-Biphenyl]-3-yl]oxy]ethyl]-3-(1-piperazinyl)-1H-pyrazin-2-one
 651046-62-7P, 3-(1-Piperazinyl)-1-[2-(2,3,4-trifluorophenoxy)ethyl]-1H-pyrazin-2-one
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 651046-64-9P, 1-[2-[(1,3-Benzodioxol-5-yl)oxy]ethyl]-3-(1-piperazinyl)-1H-pyrazin-2-one
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 trifluoroacetate 651047-03-9P, 1-[2-(3-Methoxyphenylthio)ethyl]-3-(1-piperazinyl)-1H-pyrazin-2-one
 651047-04-0P, 1-[2-(3-Methoxyphenylthio)ethyl]-3-(1-piperazinyl)-1H-pyrazin-2-one
 trifluoroacetate 651047-05-1P, 1-[2-(4-Allyl-2-methoxyphenoxy)ethyl]-3-(1-piperazinyl)-1H-pyrazin-2-one
 651047-06-2P, 1-[2-(4-Allyl-2-methoxyphenoxy)ethyl]-3-(1-piperazinyl)-1H-pyrazin-2-one
 trifluoroacetate 651047-07-3P, 1-[2-[(5,6,7,8-Tetrahydronaphthalen-2-yl)oxy]ethyl]-3-(1-piperazinyl)-1H-pyrazin-2-one
 651047-08-4P, 1-[2-[(5,6,7,8-Tetrahydronaphthalen-2-yl)oxy]ethyl]-3-(1-piperazinyl)-1H-pyrazin-2-one
 trifluoroacetate 651047-09-5P, 1-[2-(2,6-Difluorophenoxy)ethyl]-3-(3-methyl-1-piperazinyl)-1H-pyrazin-2-one
 651047-10-8P,

1-[2-(2,6-Difluorophenoxy)ethyl]-3-(3-methyl-1-piperazinyl)-1H-pyrazin-2-one trifluoroacetate 651047-11-9P, 1-[2-(4-Trifluoromethylphenoxy)ethyl]-3-(3-methyl-1-piperazinyl)-1H-pyrazin-2-one 651047-12-0P, 1-[2-(4-Trifluoromethylphenoxy)ethyl]-3-(3-methyl-1-piperazinyl)-1H-pyrazin-2-one trifluoroacetate 651047-13-1P, 1-[2-(4-Bromophenoxy)ethyl]-3-(3-methyl-1-piperazinyl)-1H-pyrazin-2-one 651047-14-2P, 1-[2-(4-Bromophenoxy)ethyl]-3-(3-methyl-1-piperazinyl)-1H-pyrazin-2-one trifluoroacetate 651047-15-3P, 1-[2-(Phenoxy)ethyl]-3-(3-methyl-1-piperazinyl)-1H-pyrazin-2-one 651047-16-4P, 1-[2-(Phenoxy)ethyl]-3-(3-methyl-1-piperazinyl)-1H-pyrazin-2-one trifluoroacetate 651047-17-5P, 1-[2-(2,4,5-Trifluorophenoxy)ethyl]-3-(3-methyl-1-piperazinyl)-1H-pyrazin-2-one 651047-18-6P, 1-[2-(2,4,5-Trifluorophenoxy)ethyl]-3-(3-methyl-1-piperazinyl)-1H-pyrazin-2-one trifluoroacetate 651047-19-7P, 1-[2-(2,4,5-Trifluorophenoxy)ethyl]-3-(1,4-diazepan-1-yl)-1H-pyrazin-2-one 651047-20-0P, 1-[2-(2,4,5-Trifluorophenoxy)ethyl]-3-(1,4-diazepan-1-yl)-1H-pyrazin-2-one trifluoroacetate 651047-21-1P, 1-[2-(4-Fluorophenoxy)ethyl]-3-(1,4-diazepan-1-yl)-1H-pyrazin-2-one 651047-22-2P, 1-[2-(4-Fluorophenoxy)ethyl]-3-(1,4-diazepan-1-yl)-1H-pyrazin-2-one trifluoroacetate 651047-23-3P, 1-[2-(4-Isopropylphenoxy)ethyl]-3-(1,4-diazepan-1-yl)-1H-pyrazin-2-one 651047-24-4P, 1-[2-(4-Isopropylphenoxy)ethyl]-3-(1,4-diazepan-1-yl)-1H-pyrazin-2-one trifluoroacetate 651047-25-5P, 1-[2-(2-Methylthiophenoxy)ethyl]-3-(1,4-diazepan-1-yl)-1H-pyrazin-2-one 651047-26-6P, 1-[2-[2-(Methylthio)phenoxy]ethyl]-3-(1,4-diazepan-1-yl)-1H-pyrazin-2-one trifluoroacetate 651047-27-7P, 1-(2,4,5-Trifluorobenzyl)-3-(1-piperazinyl)-1H-pyrazin-2-one 651047-28-8P, 1-(2,4,5-Trifluorobenzyl)-3-(1-piperazinyl)-1H-pyrazin-2-one trifluoroacetate 651047-31-3P, 1-[3-(2,4,5-Trifluorophenyl)propyl]-3-(1-piperazinyl)-1H-pyrazin-2-one 651047-32-4P, 1-[3-(2,4,5-Trifluorophenyl)propyl]-3-(1-piperazinyl)-1H-pyrazin-2-one trifluoroacetate 651047-36-8P, 1-[(2,3-Dihydrobenzo[1,4]dioxin-2-yl)methyl]-3-(1-piperazinyl)-1H-pyrazin-2-one 651047-37-9P, 1-[(2,3-Dihydrobenzo[1,4]dioxin-2-yl)methyl]-3-(1-piperazinyl)-1H-pyrazin-2-one trifluoroacetate 651047-39-1P, 3-(Piperazin-1-yl)-1-[2-(2,4,5-trifluorophenoxy)ethyl]-1H-quinoxalin-2-one 651047-40-4P, 3-(Piperazin-1-yl)-1-[2-(2,4,5-trifluorophenoxy)ethyl]-1H-quinoxalin-2-one trifluoroacetate 651047-45-9P, 1-[2-(2,4,5-Trifluorophenoxy)ethyl]-3-(4-n-butyl-1-piperazinyl)-1H-pyrazin-2-one 651047-47-1P, 1-[2-(2,4,5-Trifluorophenoxy)ethyl]-3-[4-(2-methoxyethyl)-1-piperazinyl]-1H-pyrazin-2-one 651047-48-2P, 1-[2-(2,4,5-Trifluorophenoxy)ethyl]-3-[4-(2-methoxyethyl)-1-piperazinyl]-1H-pyrazin-2-one trifluoroacetate 651047-49-3P, 1-[2-(2,4,5-Trifluorophenoxy)ethyl]-3-(4-methyl-1-piperazinyl)-1H-pyrazin-2-one 651047-52-8P, 1-[2-(2,4,5-Trifluorophenoxy)ethyl]-3-(4-isopropyl-1-piperazinyl)-1H-pyrazin-2-one 651047-55-1P, 1-[2-[(5-Methyl-[1,2,4]triazolo[1,5-a]pyrimidin-7-yl)oxy]ethyl]-3-(1-piperazinyl)-1H-pyrazin-2-one hydrochloride 651047-57-3P, 1-[2-(4-Cyanophenoxy)ethyl]-3-(1-piperazinyl)-1H-pyrazin-2-one maleate 651047-59-5P, 1-[4-(2,4,5-Trifluorophenoxy)butyl]-3-(1-piperazinyl)-1H-pyrazin-2-one 651047-60-8P, 1-[4-(2,4,5-Trifluorophenoxy)butyl]-3-(1-piperazinyl)-1H-pyrazin-2-one trifluoroacetate 651047-64-2P, 1-[3-(2,4,5-Trifluorophenoxy)propyl]-3-(1-piperazinyl)-1H-pyrazin-2-one 651047-65-3P, 1-[3-(2,4,5-Trifluorophenoxy)propyl]-3-(1-piperazinyl)-1H-pyrazin-2-one trifluoroacetate 651047-69-7P, 3-[4-(1-Phenylethyl)piperazin-1-yl]-1-[2-(2,4,5-trifluorophenoxy)ethyl]-1H-pyrazin-2-one hydrochloride 651047-70-0P, 3-[4-(2-Phenoxyethyl)piperazin-1-yl]-1-[2-(2,4,5-trifluorophenoxy)ethyl]-1H-pyrazin-2-one hydrochloride 651047-71-1P, 3-[4-(2-Phenylethyl)piperazin-1-yl]-1-[2-(2,4,5-trifluorophenoxy)ethyl]-1H-pyrazin-2-one hydrochloride 651047-72-2P, 3-(4-Benzylpiperazin-1-yl)-1-[2-(2,4,5-trifluorophenoxy)ethyl]-1H-pyrazin-

2-one hydrochloride 651047-73-3P, 3-((2R)-2-Methylpiperazin-1-yl)-1-[2-(2,4,5-trifluorophenoxy)ethyl]-1H-pyrazin-2-one 651047-74-4P, 3-((2R)-2-Methylpiperazin-1-yl)-1-[2-(2,4,5-trifluorophenoxy)ethyl]-1H-pyrazin-2-one trifluoroacetate 651047-76-6P, 1-[2-(4-Allyl-2-methoxyphenoxy)ethyl]-3-(piperazin-1-yl)-1H-pyrazin-2-one maleate 651047-78-8P, 3-(Piperazin-1-yl)-1-[2-(3-thienyl)ethyl]-1H-pyrazin-2-one 651047-79-9P, 3-(Piperazin-1-yl)-1-[2-(3-thienyl)ethyl]-1H-pyrazin-2-one maleate 651047-80-2P, 3-(Piperazin-1-yl)-1-[2-(2-thienyl)ethyl]-1H-pyrazin-2-one 651047-81-3P, 3-(Piperazin-1-yl)-1-[2-(2-thienyl)ethyl]-1H-pyrazin-2-one trifluoroacetate 651047-82-4P, 1-[2-(1H-Indol-3-yl)ethyl]-3-(piperazin-1-yl)-1H-pyrazin-2-one 651047-83-5P, 1-[2-(1H-Indol-3-yl)ethyl]-3-(piperazin-1-yl)-1H-pyrazin-2-one trifluoroacetate 651047-84-6P, 1-[2-[(2,3-Dihydro-1,4-benzodioxin-5-yl)oxy]ethyl]-3-(piperazin-1-yl)-1H-pyrazin-2-one 651047-85-7P, 1-[2-[(2,3-Dihydro-1,4-benzodioxin-5-yl)oxy]ethyl]-3-(piperazin-1-yl)-1H-pyrazin-2-one trifluoroacetate 651047-87-9P, 1-[2-(Phenylthio)ethyl]-3-(piperazin-1-yl)-1H-pyrazin-2-one 651047-88-0P, 1-[2-(Phenylthio)ethyl]-3-(piperazin-1-yl)-1H-pyrazin-2-one trifluoroacetate 651047-89-1P, 1-(3-Oxo-3-phenylpropyl)-3-(piperazin-1-yl)-1H-pyrazin-2-one 651047-90-4P, 1-(3-Oxo-3-phenylpropyl)-3-(piperazin-1-yl)-1H-pyrazin-2-one trifluoroacetate 651047-91-5P, 1-[3-(4-Fluorophenyl)-3-oxopropyl]-3-(piperazin-1-yl)-1H-pyrazin-2-one 651047-92-6P, 1-[3-(4-Fluorophenyl)-3-oxopropyl]-3-(piperazin-1-yl)-1H-pyrazin-2-one trifluoroacetate 651047-96-0P, 1-[2-(2-Fluoro-4-nitrophenoxy)ethyl]-3-(1-piperazinyl)-1H-pyrazin-2-one 651047-97-1P, 1-[2-[(2-Oxo-2H-chromen-7-yl)oxy]ethyl]-3-(1-piperazinyl)-1H-pyrazin-2-one 651047-98-2P, 3-(1-Piperazinyl)-1-[2-(2,3,5,6-tetrafluorophenoxy)ethyl]-1H-pyrazin-2-one 651047-99-3P, 1-[2-(2,3,4,5,6-Pentafluorophenoxy)ethyl]-3-(1-piperazinyl)-1H-pyrazin-2-one 651048-00-9P, 1-[2-[(Benzisoxazol-3-yl)oxy]ethyl]-3-(1-piperazinyl)-1H-pyrazin-2-one 651048-01-0P, 3-(1-Piperazinyl)-1-[2-[(6-quinoxalinyloxy)ethyl]-1H-pyrazin-2-one 651048-03-2P, 1-[2-[(5-Methyl-[1,2,4]triazolo[1,5-a]pyrimidin-7-yl)oxy]ethyl]-3-(1-piperazinyl)-1H-pyrazin-2-one 651048-04-3P, 3-[4-(1-Phenylethyl)piperazin-1-yl]-1-[2-(2,4,5-trifluorophenoxy)ethyl]-1H-pyrazin-2-one 651048-05-4P, 3-[4-(2-Phenoxyethyl)piperazin-1-yl]-1-[2-(2,4,5-trifluorophenoxy)ethyl]-1H-pyrazin-2-one

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation);

USES (Uses)

(5-HT2A receptor **modulator**; preparation of piperazinylpyrazinones for treatment of 5-HT2A receptor-related disorders)

IT 651047-55-1P, 1-[2-[(5-Methyl-[1,2,4]triazolo[1,5-a]pyrimidin-7-yl)oxy]ethyl]-3-(1-piperazinyl)-1H-pyrazin-2-one hydrochloride 651048-03-2P, 1-[2-[(5-Methyl-[1,2,4]triazolo[1,5-a]pyrimidin-7-yl)oxy]ethyl]-3-(1-piperazinyl)-1H-pyrazin-2-one

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation);

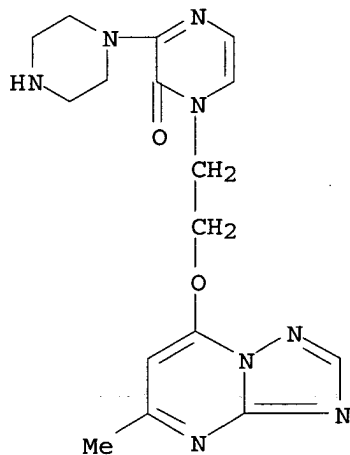
USES (Uses)

(5-HT2A receptor **modulator**; preparation of piperazinylpyrazinones for treatment of 5-HT2A receptor-related disorders)

RN 651047-55-1 HCAPLUS

CN 2(1H)-Pyrazinone, 1-[2-[(5-methyl[1,2,4]triazolo[1,5-a]pyrimidin-7-yl)oxy]ethyl]-3-(1-piperazinyl)-, monohydrochloride (9CI) (CA INDEX NAME)

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RN      651048-03-2   HCAPLUS
CN      2(1H)-Pyrazinone, 1-[2-[(5-methyl[1,2,4]triazolo[1,5-a]pyrimidin-7-yl)oxy]ethyl]-3-(1-piperazinyl)- (9CI)  (CA INDEX NAME)
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L24 ANSWER 2 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2004:41501 HCAPLUS
DOCUMENT NUMBER: 140:87744
TITLE: Affinity small molecules for the EPO receptor
INVENTOR(S): Olsson, Lennart; Naranda, Tatjana
PATENT ASSIGNEE(S): Receptron, Inc., USA
SOURCE: PCT Int. Appl., 85 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004005323	A2	20040115	WO 2003-US21394	20030703
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				

PRIORITY APPLN. INFO.: US 2002-393360P P 20020703
 US 2002-393361P P 20020703
 US 2002-394110P P 20020703

OTHER SOURCE(S): MARPAT 140:87744

AB Compds. are provided that complex with the modulating domain of erythropoietin receptor (EPO-R) for use with EPO-R to determine the presence of EPO-R, the ability of other mols. to bind to the modulating domain in competitive assays and to induce a signal by EPO-R into a cell when bound by the subject compds. in a physiol. environment. The compds. are characterized by having a six-membered heterocyclic ring comprising at least one nitrogen atom and include substituted triazolopyrimidine, pyridazinone, pyridine and piperidine.

IC ICM C07K

CC 1-12 (Pharmacology)

Section cross-reference(s): 2

IT Proteins

RL: BSU (Biological study, unclassified); BIOL (Biological study) (Bcl-xL, expression; affinity small mols. for erythropoietin (EPO) receptor and EPO receptor modulating sequence in relation to modulating the response to the stimulus of **hematopoietic** or **neuronal** cells and treatment of **anemia**)

IT Peptides, biological studies

RL: BSU (Biological study, unclassified); BUU (Biological use, unclassified); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (EPO receptor modulating sequence; affinity small mols. for erythropoietin (EPO) receptor and EPO receptor modulating sequence in relation to modulating the response to the stimulus of **hematopoietic** or **neuronal** cells and treatment of **anemia**)

IT Cell membrane

(EPO receptors of; affinity small mols. for erythropoietin (EPO) receptor and EPO receptor modulating sequence in relation to modulating the response to the stimulus of **hematopoietic** or **neuronal** cells and treatment of **anemia**)

IT **Anemia** (disease)

Cell proliferation

Combinatorial library

Drug delivery systems

Drug screening

Erythrocyte

Erythropoiesis

Hematocrit

Hematopoietic precursor cell

Human

Reticulocyte

(affinity small mols. for erythropoietin (EPO) receptor and EPO receptor modulating sequence in relation to modulating the response to the stimulus of **hematopoietic** or **neuronal** cells and treatment of **anemia**)

IT Erythropoietin receptors

RL: BSU (Biological study, unclassified); BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)
(affinity small mols. for erythropoietin (EPO) receptor and EPO receptor modulating sequence in relation to modulating the response to the stimulus of **hematopoietic** or **neuronal** cells and treatment of **anemia**)

IT Nerve

(**neuron**; affinity small mols. for erythropoietin (EPO) receptor and EPO receptor modulating sequence in relation to modulating the response to the stimulus of **hematopoietic** or **neuronal** cells and treatment of **anemia**)

IT Cytoprotective agents

(neuroprotective; affinity small mols. for erythropoietin (EPO) receptor and EPO receptor modulating sequence in relation to modulating the response to the stimulus of **hematopoietic** or **neuronal** cells and treatment of **anemia**)

IT 2503-56-2 40775-78-8 51646-16-3

51646-17-4 51646-19-6 51646-43-6

56347-20-7 63901-48-4 90559-98-1 90815-61-5

113967-71-8 113967-74-1 194342-06-8

212074-47-0 244167-89-3 245082-87-5

245413-82-5 259683-29-9 261704-08-9

261704-09-0 262291-81-6 263267-38-5

287728-46-5 303145-64-4 303145-73-5 338793-16-1

645337-19-5 645337-20-8 645337-21-9 645337-22-0

645337-23-1 645337-24-2 645337-25-3

RL: BSU (Biological study, unclassified); BUU (Biological use, unclassified); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(affinity small mols. for erythropoietin (EPO) receptor and EPO receptor **modulating** sequence in relation to **modulating** the response to the stimulus of **hematopoietic** or **neuronal** cells and treatment of **anemia**)

IT 11096-26-7, Erythropoietin

RL: BSU (Biological study, unclassified); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(affinity small mols. for erythropoietin (EPO) receptor and EPO receptor modulating sequence in relation to modulating the response to the stimulus of **hematopoietic** or **neuronal** cells and treatment of **anemia**)

IT 2503-56-2 40775-78-8 51646-16-3

51646-17-4 51646-19-6 51646-43-6

56347-20-7 90559-98-1 90815-61-5

113967-71-8 113967-74-1 194342-06-8

212074-47-0 244167-89-3 245082-87-5

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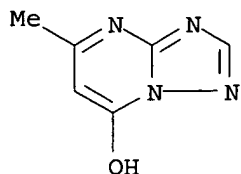
645337-21-9

RL: BSU (Biological study, unclassified); BUU (Biological use, unclassified); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(affinity small mols. for erythropoietin (EPO) receptor and EPO receptor **modulating** sequence in relation to **modulating** the response to the stimulus of **hematopoietic** or **neuronal** cells and treatment of **anemia**)

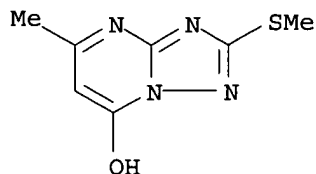
RN 2503-56-2 HCAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidin-7-ol, 5-methyl- (9CI) (CA INDEX NAME)



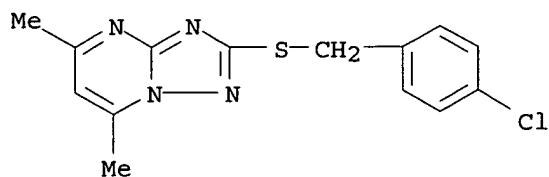
RN 40775-78-8 HCAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidin-7-ol, 5-methyl-2-(methylthio)- (9CI) (CA INDEX NAME)



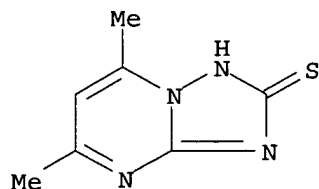
RN 51646-16-3 HCAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidine, 2-[[4-(4-chlorophenyl)methyl]thio]-5,7-dimethyl- (9CI) (CA INDEX NAME)



RN 51646-17-4 HCAPLUS

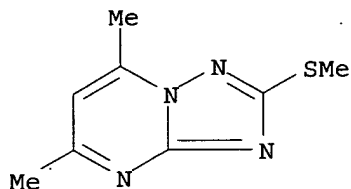
CN [1,2,4]Triazolo[1,5-a]pyrimidine-2(1H)-thione, 5,7-dimethyl- (9CI) (CA INDEX NAME)



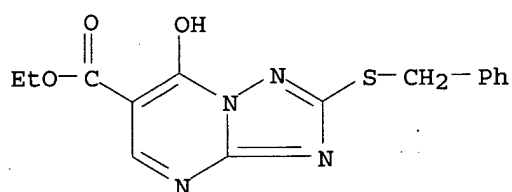
RN 51646-19-6 HCAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidine, 5,7-dimethyl-2-(methylthio)- (9CI) (CA INDEX NAME)

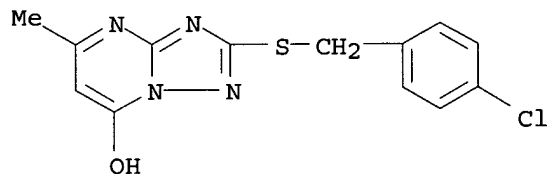
INDEX NAME)



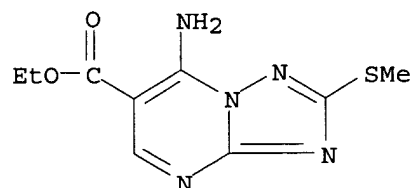
RN 51646-43-6 HCAPLUS
CN [1,2,4]Triazolo[1,5-a]pyrimidine-6-carboxylic acid, 7-hydroxy-2-
[(phenylmethyl)thio]-, ethyl ester (9CI) (CA INDEX NAME)



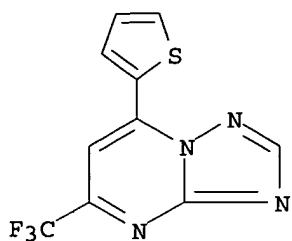
RN 56347-20-7 HCAPLUS
CN [1,2,4]Triazolo[1,5-a]pyrimidin-7-ol, 2-[[(4-chlorophenyl)methyl]thio]-5-
methyl- (9CI) (CA INDEX NAME)



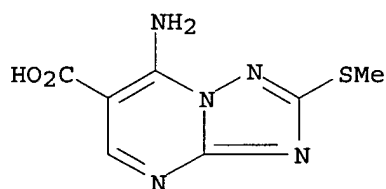
RN 90559-98-1 HCAPLUS
CN [1,2,4]Triazolo[1,5-a]pyrimidine-6-carboxylic acid, 7-amino-2-(methylthio)-
, ethyl ester (9CI) (CA INDEX NAME)



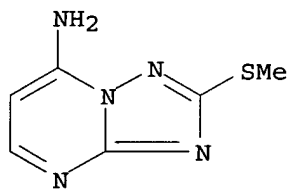
RN 90815-61-5 HCAPLUS
CN [1,2,4]Triazolo[1,5-a]pyrimidine, 7-(2-thienyl)-5-(trifluoromethyl)- (9CI)
(CA INDEX NAME)



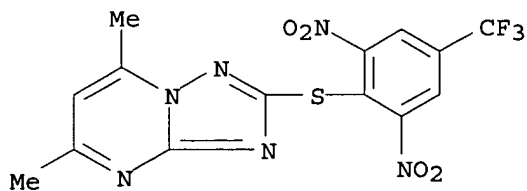
RN 113967-71-8 HCAPLUS
CN [1,2,4]Triazolo[1,5-a]pyrimidine-6-carboxylic acid, 7-amino-2-(methylthio)-
(9CI) (CA INDEX NAME)



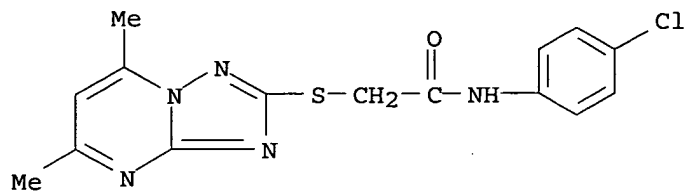
RN 113967-74-1 HCAPLUS
CN [1,2,4]Triazolo[1,5-a]pyrimidin-7-amine, 2-(methylthio)- (9CI) (CA INDEX
NAME)



RN 194342-06-8 HCAPLUS
CN [1,2,4]Triazolo[1,5-a]pyrimidine, 2-[[2,6-dinitro-4-(trifluoromethyl)phenyl]thio]-5,7-dimethyl- (9CI) (CA INDEX NAME)

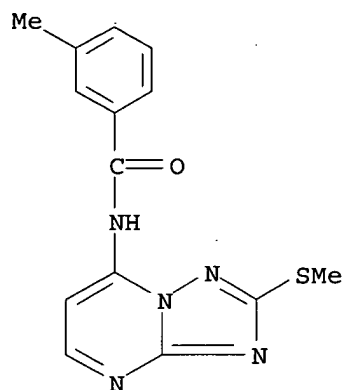


RN 212074-47-0 HCAPLUS
CN Acetamide, N-(4-chlorophenyl)-2-[(5,7-dimethyl[1,2,4]triazolo[1,5-a]pyrimidin-2-yl)thio]- (9CI) (CA INDEX NAME)



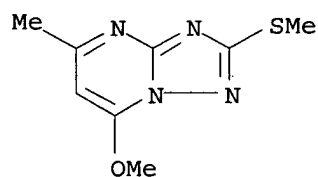
RN 244167-89-3 HCAPLUS

CN Benzamide, 3-methyl-N-[2-(methylthio)[1,2,4]triazolo[1,5-a]pyrimidin-7-yl]-(9CI) (CA INDEX NAME)



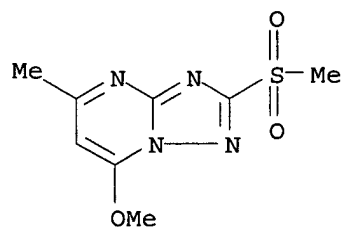
RN 245082-87-5 HCAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidine, 7-methoxy-5-methyl-2-(methylthio)-(9CI) (CA INDEX NAME)



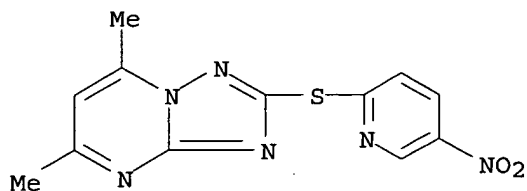
RN 245413-82-5 HCAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidine, 7-methoxy-5-methyl-2-(methylsulfonyl)-(9CI) (CA INDEX NAME)



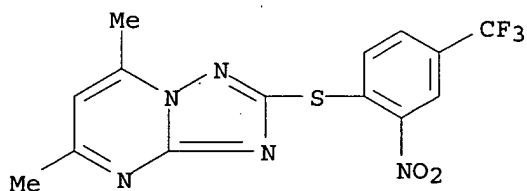
RN 261704-08-9 HCAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidine, 5,7-dimethyl-2-[(5-nitro-2-pyridinyl)thio]- (9CI) (CA INDEX NAME)



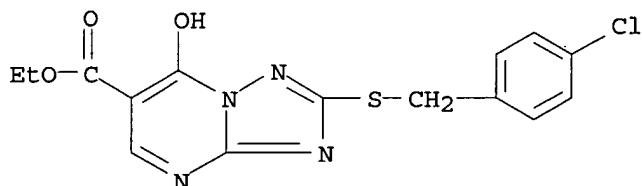
RN 261704-09-0 HCAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidine, 5,7-dimethyl-2-[[2-nitro-4-(trifluoromethyl)phenyl]thio]- (9CI) (CA INDEX NAME)



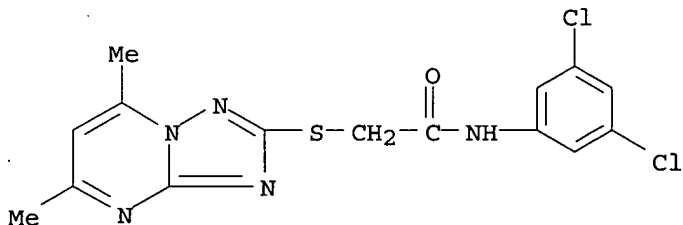
RN 262291-81-6 HCAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidine-6-carboxylic acid, 2-[[[4-chlorophenyl)methyl]thio]-7-hydroxy-, ethyl ester (9CI) (CA INDEX NAME)



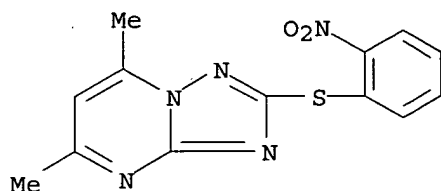
RN 263267-38-5 HCAPLUS

CN Acetamide, N-(3,5-dichlorophenyl)-2-[(5,7-dimethyl[1,2,4]triazolo[1,5-a]pyrimidin-2-yl)thio]- (9CI) (CA INDEX NAME)

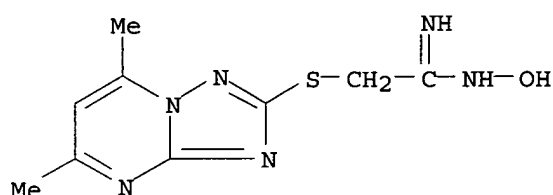


RN 287728-46-5 HCAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidine, 5,7-dimethyl-2-[(2-nitrophenyl)thio]- (9CI) (CA INDEX NAME)



RN 645337-21-9 HCAPLUS
 CN Ethanimidamide, 2-[(5,7-dimethyl[1,2,4]triazolo[1,5-a]pyrimidin-2-yl)thio]-N-hydroxy- (9CI) (CA INDEX NAME)



L24 ANSWER 3 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 2004:20322 HCAPLUS
 DOCUMENT NUMBER: 140:87658
 TITLE: Peptidomimetic modulators of cell adhesion
 INVENTOR(S): Gour, Barbara J.; Blaschuk, Orest W.; Ali, Anmar; Ni, Feng; Chen, Zhigang; Michaud, Stephanie Denise; Wang, Shaomeng; Hu, Zengjian
 PATENT ASSIGNEE(S): Can.
 SOURCE: U.S. Pat. Appl. Publ., 280 pp., Cont.-in-part of U.S. Ser. No. 6,982.
 CODEN: USXXCO
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 14
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2004006011	A1	20040108	US 2003-425557	20030428
US 6031072	A	20000229	US 1997-893534	19970711
US 6326352	B1	20011204	US 2000-507102	20000217
US 2002168761	A1	20021114	US 2001-769145	20010124
US 2002151475	A1	20021017	US 2001-6982	20011204
PRIORITY APPLN. INFO.:			US 1996-21612P	P 19960712
			US 1997-893534	A1 19970711
			US 2000-491078	B2 20000124
			US 2000-507102	A1 20000217
			US 2001-769145	B2 20010124
			US 2001-6982	A2 20011204

OTHER SOURCE(S): MARPAT 140:87658
 AB Peptidomimetics of cyclic peptides, and compns. comprising such peptidomimetics are provided. The peptidomimetics have a three-dimensional structure that is substantially similar to a

three-dimensional structure of a cyclic peptide that comprises a cadherin cell adhesion recognition sequence HAV. Methods for using such peptidomimetics for modulating cadherin-mediated cell adhesion in a variety of contexts are also provided.

IC ICM A61K038-00

NCL 514009000

CC 1-3 (Pharmacology)

Section cross-reference(s): 34, 63

IT 57-88-5D, Cholest-5-en-3-ol (3 β)-, glycoside derivs. 135-16-0,
L-Glutamic acid, N-[4-[(2-amino-1,4,5,6,7,8-hexahydro-4-oxo-6-
pteridiny]methyl]amino]benzoyl]- 487-49-0, Ethanone,
1-(2,4-dihydroxyphenyl)-2-(4-methoxyphenyl)- 548-73-2,
2H-Benzimidazol-2-one, 1-[1-[4-(4-fluorophenyl)-4-oxobutyl]-1,2,3,6-
tetrahydro-4-pyridinyl]-1,3-dihydro- 570-88-7, Cholest-4-ene-3,6-diol,
(3 β ,6 β)- 1210-66-8, 1H-Purin-6-amine, N-phenyl- 1482-74-2,
2-Propen-1-one, 3-phenyl-1-(2,3,4-trihydroxyphenyl)- 1699-40-7,
Benzeneacetamide, 4-methoxy-N-[2-[3-methoxy-4-(phenylmethoxy)phenyl]ethyl]-
3-(phenylmethoxy)- 1776-30-3, 2-Propen-1-one, 1-(2,4-dihydroxyphenyl)-3-
phenyl- 2486-02-4, Benzoic acid, 3,4,5-trihydroxy-, 3-methylbutyl ester
2810-37-9, 1H-Isoindole-1,3(2H)-dione, 2-[5-(1H-benzotriazol-1-yl)propyl]-
2979-51-3, 1H-Imidazole, 1-(1-oxo-3-phenyl-2-propenyl)- 3242-68-0,
L-Glutamic acid, N-[4-[[2-[(2-amino-1,4-dihydro-4-oxo-5-
pyrimidinyl)amino]ethyl]amino]benzoyl]- 3257-73-6, 9H-Purin-6-amine,
9-[2,3,5-tris-O-(phenylmethyl)- β -D-arabinofuranosyl]- 3561-56-6,
L-Asparagine, N2-[(phenylmethoxy)carbonyl]-, (4-nitrophenyl)methyl ester
3566-25-4, L-Glutamic acid, N-[4-[[2-(2-amino-1,4-dihydro-4-oxo-6-
pteridiny]ethyl]amino]benzoyl]- 3575-07-3, 1H-Benzimidazole,
2,2'-(1,2-ethanediyl)bis- 3922-47-2, 1H-1,2,4-Triazol-3-amine,
5-[(phenylmethyl)thio]- 4672-96-2, Benzeneacetamide,
3-methoxy-N-[2-[4-methoxy-3-(phenylmethoxy)phenyl]ethyl]-4-(phenylmethoxy)-
5226-71-1, Benzene, 1,1'-[1,10-decanediylbis(oxy)]bis[3-nitro-
5341-00-4, 1,4-Naphthalenedione, 2-[3-(decahydro-2-naphthalenyl)propyl]-3-
hydroxy- 5415-88-3, 1H-Purine-2,6-dione, 3,7-dihydro-1,3,7-trimethyl-8-
(4-phenylbutoxy)- 5421-95-4, Urea, (3-phenyl-1,2,4-oxadiazol-5-yl)-
5426-87-9, Benzamide, N-[(2,3,6,7-tetrahydro-1,3-dimethyl-2,6-dioxo-1H-
purin-8-yl)methyl]- 5429-46-9, Benzamide, N-[2-(2,3,6,7-tetrahydro-1,3-
dimethyl-2,6-dioxo-1H-purin-8-yl)ethyl]- 5446-36-6, 1H-Purin-6-amine,
N-(4-methylphenyl)- 5454-50-2, Ethanone, 1-phenyl-2-(1H-purin-6-ylthio)-
5454-52-4, 1H-Purine, 6-[(2-phenoxyethyl)thio]- 5508-58-7,
2(3H)-Furanone, 3-[2-[(1R,4aS,5R,6R,8aS)-decahydro-6-hydroxy-5-
(hydroxymethyl)-5,8a-dimethyl-2-methylene-1-naphthalenyl]ethylidene]dihydr
o-4-hydroxy-, (3E,4S)- 5534-95-2 5800-34-0, Pentanoic acid,
5-[[[(1S)-2-[(4-nitrophenyl)amino]-2-oxo-1-(phenylmethyl)ethyl]amino]-5-oxo-
6286-57-3, 5(4H)-Isoxazolone, 4-(1,3-benzodioxol-5-ylmethylene)-3-
phenyl- 6295-27-8, 7H-1,2,3-Triazolo[4,5-d]pyrimidin-7-one,
5-amino-2,6-dihydro-2-phenyl- 6300-80-7, Benzaldehyde,
4-(dimethylamino)-, 7H-purin-6-ylhydrazone 6320-71-4,
1,4-Naphthalenedione, 2-(4-cyclohexylbutyl)-3-hydroxy- 6322-09-4,
2(1H)-Quinoxalinone, 3-[2-(2-chlorophenyl)ethenyl]-7-methyl- 6323-88-2,
2(1H)-Quinoxalinone, 3-[2-(3-nitrophenyl)ethenyl]- 6323-89-3,
2(1H)-Quinoxalinone, 3-(2-phenylethenyl)- 6331-03-9, Benzaldehyde,
4-nitro-, 7H-purin-6-ylhydrazone 6338-84-7, 1H-Purine-2,6-dione,
3,7-dihydro-1,3,7-trimethyl-8-(2-phenylethyl)- 6340-76-7,
2,4-Pyrimidinediamine, 6-chloro-N4-(3-methylphenyl)- 6633-66-5,
2,4,6-Pyrimidinetriamine, N4-(4-bromophenyl)- 6807-82-5, L-Glutamic
acid, N-[4-[[[(2-amino-1,4-dihydro-4-oxo-6-pteridiny]methyl]amino]benzoyl]-
L- α -glutamyl- 6962-62-5, 2-Propen-1-one, 3-(1,3-benzodioxol-5-yl)-
1-(2,4-dihydroxyphenyl)- 6975-34-4, 1H-Purine, 6-[(3-phenyl-2-
propenyl)thio]- 7781-29-5, 2,4-Pyrimidinediamine, 6-methyl-N4-phenyl-

10320-97-5, 1,2,3,4-Thiatriazol-5-amine, N-1-naphthalenyl- 13184-14-0,
 L-Lysine, L-lysyl-L-lysyl- 13351-10-5, 2-Propen-1-one,
 1-(2,4-dihydroxyphenyl)-3-(4-methoxyphenyl)- 13745-20-5, 2-Propen-1-one,
 1-(2,4-dihydroxyphenyl)-3-(4-hydroxyphenyl)- 15013-60-2,
 Cholest-4-ene-3,6-diol, (3 β ,6 α)- 15970-42-0,
 1H-Imidazole-1,2-diamine, 4-(4-chlorophenyl)- 16856-21-6, L-Tryptophan,
 N-[N-[(phenylmethoxy)carbonyl]-L-phenylalanyl]-, methyl ester
 16879-84-8, L-Threonine, N-[(phenylmethoxy)carbonyl]-,
 (4-nitrophenyl)methyl ester 17357-75-4, 1H-1,2,4-Triazole,
 3-[[[(4-methoxyphenyl)methyl]thio]- 17430-65-8, L-Tryptophan,
 N-[(phenylmethoxy)carbonyl]-L-valyl-, methyl ester 17496-31-0,
 1H-Imidazole, 4-[[[(phenylmethyl)thio]methyl]- 18100-11-3,
 1,4-Naphthalenedione, 2-(3-cyclohexylbutyl)-3-hydroxy- 18100-12-4,
 1,4-Naphthalenedione, 2-[3-(4-chlorophenyl)propyl]-3-hydroxy-
 18211-37-5, 1,4-Naphthalenedione, 2-hydroxy-3-[3-(4-methylphenyl)propyl]-
 19312-13-1, 2-Propen-1-one, 1-(2,5-dihydroxyphenyl)-3-phenyl-
 19484-75-4D, 2H-1-Benzopyran-2-one, 3,4-dihydro-7-hydroxy-4-methyl-,
 furanoxide derivative 19889-31-7, 1H-Imidazole-4-propanamide,
 α -amino-N-2-naphthalenyl- 20621-49-2, 2-Propen-1-one,
 1-(2,6-dihydroxy-4-methoxyphenyl)-3-(4-methoxyphenyl)- 20711-05-1,
 L-Glutamic acid, N-[4-[[2-(2-amino-1,5,6,7-tetrahydro-4-hydroxy-6-
 pteridiny]ethyl)amino]benzoyl]- 21108-76-9, Imidazo[2,1-b]thiazol-3(2H)-
 one, 5,6-dihydro-2-(3-phenyl-2-propenylidene)- 21658-45-7, Glycine,
 L-arginyl-L-prolyl-L-prolyl- 23567-67-1, Phenol, 4-(1,2,3,4-thiatriazol-
 5-ylamino)- 23815-88-5, 1-6-Bradykinin 24205-32-1, L-Glutamic acid,
 N-[4-[[2-(2,4-diamino-5-methyl-6-quinazolinyl)methyl]amino]benzoyl]-
 , diethylester 24386-39-8, Urea, N-1-naphthalenyl-N'-2-pyrimidinyl-
 24829-12-7, Phenol, 2-[(1H-1,2,4-triazol-3-ylimino)methyl]- 26962-50-5,
 2-Propen-1-one, 1-(2,4-dihydroxyphenyl)-3-(2-hydroxyphenyl)- 27069-81-4,
 L-Glutamic acid, N-[4-[[2-(2-amino-1,4-dihydro-4-oxo-6-
 quinazolinyl)methyl]amino]benzoyl]-, diethyl ester 27430-15-5,
 4,6(1H,5H)-Pyrimidinedione, 5-[[4-(dimethylamino)phenyl]methylene]dihydro-
 2-thioxo- 27430-17-7, 4,6(1H,5H)-Pyrimidinedione, dihydro-5-(3-phenyl-2-
 propenylidene)-2-thioxo- 28005-33-6, Benzene, 1,1'-methylenebis[4-[(4-
 nitrophenyl)thio]- 28246-23-3, Ethanone, 2-(1H-imidazol-2-ylthio)-1-
 phenyl- 28772-56-7, 2H-1-Benzopyran-2-one, 3-[3-(4'-bromo[1,1'-biphenyl]-
 4-yl)-3-hydroxy-1-phenylpropyl]-4-hydroxy- 29654-52-2, Benzene,
 1,1'-methylenebis[4-[(4-nitrophenyl)sulfonyl]- 30148-18-6, Methanone,
 (4-chlorophenyl)(1-methyl-1H-imidazol-2-yl)- 30216-31-0D, Benzoxazole,
 2-[2-(2-chlorophenyl)ethenyl]-, derivs. 30355-60-3, 1,3,5-Triazine-2,4-
 diamine, 6-(chloromethyl)-N-phenyl- 30826-46-1, L-Glutamic acid,
 N-[4-[[[5,7-bis(acetylamino)pyrido[3,4-b]pyrazin-3-
 yl]methyl]methylamino]benzoyl]-, diethyl ester 30826-47-2, L-Glutamic
 acid, N-[4-[[[6,8-bis(acetylamino)pyrido[2,3-b]pyrazin-2-
 yl]methyl]methylamino]benzoyl]-, diethyl ester 33254-46-5,
 6H-Purine-6-thione, 1,9-dihydro-9-(3-phenylpropyl)- 34396-76-4,
 6H-Purin-6-one, 1,9-dihydro-9-(3-phenylpropyl)- 37664-31-6, Ethanone,
 1-(4-chlorophenyl)-2-(1H-1,2,4-triazol-3-ylthio)- 40538-65-6,
 5(4H)-Isoxazolone, 3-methyl-4-[(phenylamino)methylene]- 40816-36-2,
 4,6-Pyrimidinediamine, 5-nitro-N-phenyl- 41266-78-8,
 1H-1,2,4-Triazol-3-amine, 5-[[[(4-chlorophenyl)methyl]thio]- 41600-13-9,
 L-Glutamic acid, N-[4-[[[2-(2,4-diamino-6-pteridiny]methyl]methylamino]benzo
 yl]-L- γ -glutamyl- 42220-83-7, 2-Propen-1-one, 1-(2,4-
 dihydroxyphenyl)-3-(3-hydroxyphenyl)- 46825-86-9, Pyrimidinetetramine,
 N4-(4-bromophenyl)- 50602-77-2, L-Glutamic acid, N-[4-[[[2-(2,4-diamino-6-
 pteridiny]methyl]methylamino]benzoyl]-, dibutyl ester 51646-15-2
 , [1,2,4]Triazolo[1,5-a]pyrimidine, 5,7-dimethyl-2-[(phenylmethyl)thio]-
 51893-98-2, Benzoic acid, 2-hydroxy-, [2-[(5-ethyl-1,4-dihydro-6-methyl-4-
 oxo-2-pyrimidinyl)thio]-1-phenylethylidene]hydrazide 51934-26-0,

L-Glutamic acid, N-[4-[[[(7-amino-1,5-dihydro-5-thioxopyrimido[5,4-e]-1,2,4-triazin-3-yl)methyl]amino]benzoyl]-, diethyl ester, monohydrochloride
 51934-28-2, L-Glutamic acid, N-[4-[[[(5,7-diaminopyrimido[5,4-e]-1,2,4-triazin-3-yl)methyl]amino]benzoyl]-, diethyl ester 54299-50-2,
 2-Propen-1-one, 1-(2,4-dihydroxy-3,6-dimethoxyphenyl)-3-phenyl-
 54395-52-7, 1H-Isoindole-1,3(2H)-dione, 5,5'-[(1-methylethylidene)bis(4,1-phenyleneoxy)]bis[2-methyl- 56025-86-6, 1H-Purine-2,6-dione,
 3,7-dihydro-3-methyl-7-(phenylmethyl)- 56307-99-4, Ethanone,
 1-(2,4-dihydroxyphenyl)-2-(phenylthio)- 57710-80-2, 1H-Benzotriazole-1-carboxylic acid, phenylmethyl ester 57808-66-9, 2H-Benzimidazol-2-one,
 5-chloro-1-[1-[3-(2,3-dihydro-2-oxo-1H-benzimidazol-1-yl)propyl]-4-piperidinyll]-1,3-dihydro- 57966-42-4, L-Threonine, L-arginyl-L-tyrosyl-L-leucyl-L-prolyl- 58677-09-1, L-Glutamic acid, N-[4-[[[(2-amino-1,4-dihydro-4-oxo-6-quinazolinyl)methyl]methylamino]benzoyl]-, diethyl ester
 60045-61-6, 4,6(1H,5H)-Pyrimidinedione, dihydro-5-[(4-methoxyphenyl)methylene]-2-thioxo- 60407-48-9, L-Isoleucine,
 L-arginylglycyl-L-prolyl-L-phenylalanyl-L-prolyl- 60482-96-4, L-Leucine,
 L-arginyl-L-prolyl-L-tyrosyl-L-isoleucyl- 61043-53-6,
 L-Phenylalaninamide, N-(3-carboxy-1-oxopropyl)-L-alanyl-L-alanyl-N-(4-nitrophenyl)- 64792-21-8, 2-Propenal, 3-phenyl-, (1,4-dihydro-6-methyl-4-oxo-2-pyrimidinyl)hydrazone 64801-58-7, L-Aspartic acid,
 N-[4-[[[(2,4-diamino-6-pteridinyll)methyl]methylamino]benzoyl]-L-γ-glutamyl- 65147-09-3, L-Argininamide, N-[(1,1-dimethylethoxy)carbonyl]-L-leucylglycyl-N-(4-methyl-2-oxo-2H-1-benzopyran-7-yl)- 65757-04-2,
 L-Glutamic acid, N-[4-[[[(1,2,3,4-tetrahydro-2-imino-1,3-dimethyl-4-oxo-6-pteridinyll)methyl]amino]benzoyl]-, dimethyl ester 65757-05-3, L-Glutamic acid, N-[4-[[[(2-amino-3,4-dihydro-3-methyl-4-oxo-6-pteridinyll)methyl]amino]benzoyl]-, dimethyl ester 65877-43-2D,
 1,3-Benzenediol, 5-[2-(3-hydroxy-4-methoxyphenyl)ethenyl]-, glycoside derivative 66048-53-1, Guanosine, 2',3',5'-tribenzoate 66147-31-7,
 L-Glutamic acid, N-[4-[[[(2,4-diamino-6-pteridinyll)methyl]methylamino]benzoyl]-, 5-butyl ester 67368-29-0, L-Alanine, L-methionyl-L-arginyl-L-phenylalanyl- 67655-19-0, Phenol, 2,2'-[(2-hydroxy-1,3-propanediyl)bis(oxy)]bis- 67836-16-2, Acetamide, 2-(2,4-dichlorophenoxy)-N-1H-1,2,4-triazol-3-yl- 68047-41-6, 1,3,4-Oxadiazole,
 2-(3-bromophenyl)-5-(2-naphthalenyl)- 68215-68-9, Phenol,
 2-[4-amino-6-[(4-chlorophenyl)amino]-1,3,5-triazin-2-yl]-4-chloro-68682-02-0, 4H-1-Benzopyran-4-one, 2,3-dihydro-5,7-dihydroxy-2-(4-hydroxyphenyl)-8-(3-methyl-2-butenyl)- 68838-40-4, 1H-1,2,4-Triazole,
 3-methyl-5-[(phenylmethyl)thio]- 69097-98-9, 4H-1-Benzopyran-4-one, 2,3-dihydro-5,7-dihydroxy-2-(4-hydroxy-3-methoxyphenyl)- 69193-20-0,
 4-Pyrimidinamine, 5-bromo-N-phenyl- 69480-15-5, 3H-1,2,4-Triazole-3-thione, 5-[4-(1,1-dimethylethyl)phenyl]-1,2-dihydro- 70280-72-7,
 L-Glutamic acid, N-[4-[[[(2,4-diamino-6-pteridinyll)methyl] (phenylmethyl)amino]benzoyl]-, diethyl ester 70280-75-0, L-Glutamic acid,
 N-[4-[[[(2,4-diamino-6-pteridinyll)methyl]ethylamino]benzoyl]-, diethyl ester 70539-54-7, L-Glutamic acid, N-[3,5-dichloro-4-[[[(2,4-diamino-6-pteridinyll)methyl]ethylamino]benzoyl]-, diethyl ester 70968-04-6,
 L-Leucinamide, N-(3-carboxy-1-oxopropyl)-L-alanyl-L-alanyl-L-prolyl-N-(4-nitrophenyl)- 71047-38-6, 1H-Imidazole, 1-(3,7-dimethyl-2,6-octadienyl)-71074-46-9, Glycine, N-[N-[4-[[[(2,4-diamino-6-pteridinyll)methyl]methylamino]benzoyl]-L-γ-glutamyl]- 71074-48-1,
 L-Aspartic acid, N-[4-[[[(2,4-diamino-6-pteridinyll)methyl]methylamino]benzoyl]-L-α-glutamyl- 71074-49-2, L-Glutamic acid,
 N-[4-[[[(2,4-diamino-6-pteridinyll)methyl]methylamino]benzoyl]-L-α-glutamyl- 71707-02-3, L-Glutamic acid, N-[N-[4-[[[(2,4-diamino-6-pteridinyll)methyl]amino]benzoyl]-L-γ-glutamyl]- 72630-15-0,
 Glutamic acid, N-[4-[[[2-(2-amino-1,4,5,6,7,8-hexahydro-5-methyl-4-oxo-6-pteridinyll)ethyl]amino]benzoyl]- 72682-77-0, L-Isoleucinamide,

N-(3-carboxy-1-oxopropyl)-L-alanyl-L-alanyl-L-prolyl-N-(4-nitrophenyl)-
 72704-76-8, 2-Propen-1-one, 3-(3,4-dihydroxyphenyl)-1-phenyl-
 73554-90-2, L-Argininamide, N-[(1,1-dimethylethoxy)carbonyl]-L-
 phenylalanyl-L-seryl-N-(4-methyl-2-oxo-2H-1-benzopyran-7-yl)-
 73572-58-4, L-Phenylalanine, N-[(1,1-dimethylethoxy)carbonyl]-L-
 phenylalanyl-L-leucyl-L-phenylalanyl-L-leucyl- 74039-67-1,
 1H-Purine-2,6-dione, 3,7-dihydro-1,3-dimethyl-8-(3-phenyl-2-propenyl)-
 74405-42-8, Adenosine, N-benzoyl-5'-O-[bis(4-methoxyphenyl)phenylmethyl]-
 2'-deoxy-, 3'-(hydrogen butanedioate) 74405-44-0, Cytidine,
 N-benzoyl-5'-O-[bis(4-methoxyphenyl)phenylmethyl]-2'-deoxy-, 3'-(hydrogen
 butanedioate) 74853-69-3, L-Leucine, N2-acetyl-L-arginyl-L-arginyl-L-
 prolyl-L-tyrosyl-L-isoleucyl- 75651-68-2, L-Phenylalaninamide,
 N-(3-carboxy-1-oxopropyl)-L-phenylalanyl-L-prolyl-N-(4-nitrophenyl)-
 75960-43-9, 1H-Imidazole-4-hexanoic acid, 5-(chloromethyl)-2,3-dihydro-
 s,2-dioxo-, ethyl ester 76172-68-4, 1-Propanone,
 3-(4-methoxyphenyl)-1-(2,4,6-trihydroxyphenyl)- 80032-99-1,
 1H-1,2,4-Triazole, 3,3'-[1,4-butanediylbis(thio)]bis- 80360-08-3,
 L-Glutamic acid, N-[4-[[[2,4-diaminopyrido[2,3-d]pyrimidin-6-
 yl)methyl]amino]benzoyl]-, diethylester 81066-61-7, 2-Pyridinamine,
 3-[[4-(1,1-dimethylethyl)phenyl]methoxy]- 81587-37-3, 3-Pyridinethiol,
 2-[(2,6-diamino-4-pyrimidinyl)amino]-6-methyl- 82628-82-8, 1-Propanone,
 3-(4-nitrophenyl)-1-(2,4,6-trihydroxyphenyl)- 82855-85-4, L-Glutamic
 acid, N-[4-[[[2-amino-1,4,5,6,7,8-hexahydro-4-oxopyrido[3,2-d]pyrimidin-6-
 yl)methyl]amino]benzoyl]-, diethyl ester 85122-85-6,
 1H-Isoindole-1,3(2H)-dione, 2,2'-[1,3-propanediylbis(4,1-
 piperidinediylmethylene)]bis- 86669-33-2, L-Glutamic acid,
 N-[4-[[[2,4-diamino-6-pteridinyl)methyl]methylamino]benzoyl]-,
 bis(1,1-dimethylethyl) ester 90259-60-2, Benzamide, 2-amino-N-[3-(1H-
 imidazol-1-yl)propyl]- 90259-61-3, Benzamide, 2-[[[4-
 chlorophenyl)sulfonyl]amino]-N-[3-(1H-imidazol-1-yl)propyl]- 92899-39-3,
 Glycine, L-valylglycyl-L-valyl-L-alanyl-L-prolyl- 92954-99-9, Glycine,
 1-acetyl-L-prolyl-L-leucylglycyl-L-leucyl-L-leucyl-, ethyl ester
 93515-01-6, L-Threonine, L-tyrosyl-L-prolyl-L-prolyl-L- α -glutamyl-L-
 prolyl-L- α -glutamyl- 93524-30-2, β -D-Glucopyranosiduronic
 acid, (3 α ,5 β)-21-(acetyloxy)-20-[(aminocarbonyl)hydrazono]pregn
 an-3-yl, methyl ester, 2,3,4-triacetate 93674-97-6, L-Serine,
 L-arginylglycyl-L- α -glutamyl- 95192-21-5, L-Phenylalaninamide,
 N-(3-carboxy-1-oxopropyl)-L-phenylalanyl-L-alanyl-N-(4-nitrophenyl)-
 95192-38-4, L-Phenylalaninamide, N-(3-carboxy-1-oxopropyl)-L-alanyl-L-
 valyl-L-prolyl-N-(4-nitrophenyl)- 95210-75-6, L-Proline,
 L-tyrosyl-L-prolyl-L-phenylalanyl-L-valyl-L- α -glutamyl-L-prolyl-L-
 isoleucyl- 98018-39-4, Ethanone, 2-[(2-amino-1H-purin-6-yl)thio]-1-
 phenyl- 98151-93-0, L-Proline, L-tyrosyl-L-prolyl-L-phenylalanyl-L-
 prolylglycyl-L-prolyl-L-isoleucyl- 100975-56-2, Benzaldehyde,
 4-hydroxy-, (2,3,6,7-tetrahydro-1,3,7-trimethyl-2,6-dioxo-1H-purin-8-
 yl)hydrazone 102212-40-8, 1H-Purine-2,6-dione, 3,7-dihydro-1,3-dimethyl-
 8-[(2-phenylethyl)amino]- 103030-49-5, 2,4-Pyrimidinediamine,
 N4-(4-chlorophenyl)-5-nitro- 103398-43-2, Benzenemethanol,
 2-[bis[2-[(4-nitrobenzoyl)oxy]ethyl]amino]-, 4-nitrobenzoate (ester)
 105037-36-3, Benzenesulfonic acid, 4-[(7-chloro-4-quinazolinyl)amino]-
 108608-63-5, Glycine, L-seryl-L- α -aspartylglycyl-L-arginyl-
 110906-89-3, L-Phenylalaninamide, N-(3-carboxy-1-oxopropyl)-L-phenylalanyl-
 L-alanyl-L-alanyl-N-(4-nitrophenyl)- 111172-14-6, 1,3-Benzodioxole-5-
 carboxaldehyde, O-(2-thienylcarbonyl)oxime 112233-74-6, Carbamic acid,
 diphenyl-, 2-(acetyl amino)-1H-purin-6-yl ester 113866-00-5,
 L-Argininamide, N-[(1,1-dimethylethoxy)carbonyl]-L- α -aspartyl-L-
 prolyl-N-(4-methyl-2-oxo-2H-1-benzopyran-7-yl)-, phenylmethyl ester
 113866-16-3, L-Argininamide, N-[(1,1-dimethylethoxy)carbonyl]-L- α -
 glutamyl-L-alanyl-N-(4-methyl-2-oxo-2H-1-benzopyran-7-yl)-, phenylmethyl

ester 117889-48-2, 1H-Tetrazole, 5-[(2,4-dichlorophenoxy)methyl]-
 118034-92-7, L-Threonine, L-histidyl-L-phenylalanyl-L-methionyl-L-prolyl-
 120225-54-9, Benzenepropanoic acid, 4-[2-[[6-amino-9-(N-ethyl- β -D-
 ribofuranuronamidosyl)-9H-purin-2-yl]amino]ethyl]- 121036-80-4,
 1,2,4-Triazin-5(2H)-one, 6-[2-(4-methylphenyl)ethenyl]-3-phenyl-
 121036-81-5, 1,2,4-Triazin-5(2H)-one, 6-[2-(4-methoxyphenyl)ethenyl]-3-
 phenyl- 124485-41-2, L-Argininamide, N-[(phenylmethoxy)carbonyl]-L-valyl-
 L-valyl-N-(4-methyl-2-oxo-2H-1-benzopyran-7-yl)- 126235-09-4,
 1H-Purine-2,6-dione, 3,7-dihydro-1,3-dimethyl-8-(2-phenylethyl)-
 128802-79-9, L-Phenylalaninamide, N-(3-carboxy-1-oxopropyl)-L-alanyl-L-
 isoleucyl-L-prolyl-N-(4-nitrophenyl)- 131061-65-9, 7H-Purine-7-butanoic
 acid, 1,2,3,6-tetrahydro-1,3-dimethyl-2,6-dioxo-8-[(phenylmethyl)amino]-,
 ethyl ester 132467-01-7, 2(1H)-Quinoxalinone, 3-[2-(2-
 chlorophenyl)ethenyl]- 133061-57-1, 2,4-Pyrimidinediamine,
 N4-(3,5-dichlorophenyl)-6-methyl- 134759-22-1, 1H-Thieno[3,4-d]imidazole-
 4-pentanamide, N-[6-[[5-[[[(3',6'-dihydroxy-3-oxospiro[isobenzofuran-
 1(3H),9'-(9H)xanthen]-5-yl)amino]thioxomethyl]amino]pentyl]amino]-6-
 oxohexyl]hexahydro-2-oxo-, (3aS,4S,6aR)- 134796-34-2, 1H-1,2,4-Triazole,
 3-[[4-(4-chlorophenyl)methyl]thio]- 137484-84-5
 , 1,3,5-Triazin-2-amine, 4-chloro-6-[3-(2-furanyl)propoxy]-N,N-dimethyl-
 137833-31-9, Myelo peptide 2 138194-56-6, 1H-Pyrrole-2,5-dione,
 1-[3-[[4-(4-oxo-1,2,3-benzotriazin-3(4H)-yl)oxy]carbonyl]phenyl]-
 138915-75-0, L-Leucine, N-acetyl-L-histidyl-L-tryptophyl-L-alanyl-L-
 valylglycyl-L-histidyl- 142206-40-4, 1H-Benzimidazole,
 2,2'-(1,3-propanediyl)bis[1-methyl- 143113-41-1, L-Valine,
 L-Histidyl-L-Alanyl 146871-70-7, 4-Quinazolinamine, N-(3-chlorophenyl)-,
 monohydrochloride 148337-06-8, Glycine, L-prolylglycyl-L-alanyl-L-
 isoleucyl-L-prolyl- 151358-70-2, 2-Propen-1-one, 1,1'-(2,6-
 pyridinediyl)bis[3-(4-hydroxyphenyl)- 152028-96-1, 1H-Imidazole,
 4-[3-[[4-(4-iodophenyl)methoxy]propyl]- 154719-25-2, L-Lysinamide,
 N-acetyl-L-tyrosyl-L-valyl-N-[(1S)-1-(carboxymethyl)-3-[(2,6-
 dimethylbenzoyl)oxy]-2-oxopropyl]-N6-[5-[(3aS,4S,6aR)-hexahydro-2-oxo-1H-
 thieno[3,4-d]imidazol-4-yl]-1-oxopentyl]- 155373-59-4,
 4H-1-Benzopyran-4-one, 3-[[4-(1H-tetrazol-5-yl)phenyl]methyl]-
 155373-72-1, 4H-1-Benzopyran-4-one, 2-phenyl-7-[4-(1H-tetrazol-5-
 yl)butoxy]- 160347-57-9D, 2(1H)-Pyrimidinone, 5-(4-pentylphenyl)-,
 derivs. 185503-97-3, L-Lysine, N6-[[4-[[4-(dimethylamino)phenyl]azo]phen-
 yl]sulfonyl]-N2-[(9H-fluoren-9-ylmethoxy)carbonyl]- 188966-22-5D,
 Phenol, 2-(2H-benzotriazol-2-yl)-4-(1,1-dimethylhexyl)-, derivs.
 191411-47-9, 1H-Imidazole-5-methanol, 1-methyl-2-[(phenylmethyl)thio]-
 194424-08-3, Glutamic acid, N-[4-[[3-(2-thienyl)-2-
 quinoxaliny]amino]benzoyl]-, dipropyl ester 195140-70-6, 1H-Imidazole,
 1-[2-(phenylmethoxy)ethyl]- 196600-87-0, Tyrosine, N-
 [(phenylmethoxy)carbonyl]norvalylglycyl-, methyl ester 197456-56-7,
 1,4-Naphthalenedione, 2-[4-(decahydro-2-naphthalenyl)butyl]-3-hydroxy-
 198488-04-9, Urea, N,N'-(3,3'-dimethyl[1,1'-biphenyl]-4,4'-diyl)bis[N'-(2-
 methylphenyl)- 198632-08-5, L-Proline, glycyl-L-arginylglycyl-L- α -
 glutamyl-L-threonyl- 199929-21-0, 1,4-Naphthalenedione,
 2-hydroxy-3-[8-(4-methylphenoxy)octyl]- 200058-34-0,
 1,4-Naphthalenedione, 2-(3-[1,1'-bicyclohexyl]-4-ylpropyl)-3-hydroxy-
 200061-22-9, Phenol, 4,4'-(1-methylethylidene)bis-, bis(3,5-
 dinitrobenzoate) 200431-98-7, 3-Pyridinemethanamine,
 N-1H-1,2,4-triazol-3-yl- 200505-51-7, Decanedioic acid,
 bis[[4-(ethoxy-3-methoxyphenyl)methylene]hydrazide] 200706-30-5,
 4H-1,2,4-Triazol-4-amine, N-[(2,3-dihydro-1H-inden-5-yl)methylene]-
 200706-45-2, 4-Imidazolidinone, 5-[(2,3-dihydro-1H-inden-5-yl)methylene]-2-
 thioxo- 201997-13-9, 1,3-Benzenediol, 4-[[[2-hydroxy-2-(4-
 nitrophenyl)ethyl]imino]methyl]- 202118-27-2, 1H-1,2,4-Triazol-3-amine,
 N-[(2-iodophenyl)methylene]- 202118-28-3, 1H-1,2,4-Triazol-3-amine,

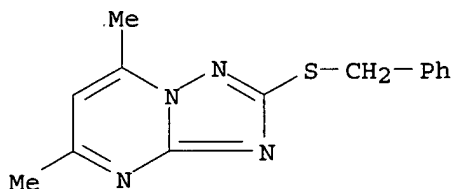
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 2-(6-methylheptyl)- 202528-15-2, Cyclo(L-alanyl-L-histidyl-L-alanyl-L-
 valyl-L- α -aspartyl-L-isoleucyl) 206360-24-9, 4H-1-Benzopyran-4-
 one, 2,3-dihydro-5,7-dihydroxy-2-(4-hydroxyphenyl)-3-(3-methyl-2-butenyl)-
 210709-22-1, L-Alanine, N2-benzoyl-L-arginyl-L-phenylalanyl-
 215434-58-5, 1-Piperazinecarbothioamide, N-3-pyridinyl-4-[4-
 (trifluoromethyl)-2-pyrimidinyl]- 215655-36-0, Benzoic acid,
 2-[[[2-[[4-(trifluoromethyl)-2-pyrimidinyl]amino]ethyl]amino]carbonyl]-
 215657-86-6, 2-Pyrrolidinone, 1-[2-hydroxy-3-[4-[4-(trifluoromethyl)-2-
 pyrimidinyl]-1-piperazinyl]propyl]- 216299-43-3, 2,5-Pyrrolidinedione,
 1-[[11-[(5-azido-1-naphthalenyl)oxy]-1-oxoundecyl]oxy]-
 RL: BSU (Biological study, unclassified); PAC (Pharmacological activity);
 PRP (Properties); THU (Therapeutic use); BIOL (Biological study)
 ; USES (Uses)

(peptidomimetic **modulators** of cadherin-mediated cell adhesion
 for therapeutic use in relation to three-dimensional structure)

IT 51646-15-2, [1,2,4]Triazolo[1,5-a]pyrimidine, 5,7-dimethyl-2-
 [(phenylmethyl)thio]-
 RL: BSU (Biological study, unclassified); PAC (Pharmacological activity);
 PRP (Properties); THU (Therapeutic use); BIOL (Biological study)
 ; USES (Uses)

(peptidomimetic **modulators** of cadherin-mediated cell adhesion
 for therapeutic use in relation to three-dimensional structure)

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 (9CI) (CA INDEX NAME)



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ACCESSION NUMBER: 2003:591184 HCAPLUS

DOCUMENT NUMBER: 139:164784

TITLE: Preparation of fused succinimides as modulators of
 nuclear hormone receptor function

INVENTOR(S): Salvati, Mark E.; Balog, James Aaron; Pickering,
 Darcia A.; Giese, Soren; Fura, Aberra; Li, Wenying;
 Patel, Ramesh N.; Hanson, Ronald L.; Mitt, Toomas;
 Roberge, Jacques; Corte, James R.; Spergel, Steven H.;
 Rampulla, Richard A.; Misra, Raj; Xiao, Hai-yun

PATENT ASSIGNEE(S): Bristol-Myers Squibb Pharma Company, USA

SOURCE: PCT Int. Appl., 763 pp.

CODEN: PIXXD2

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LANGUAGE: English

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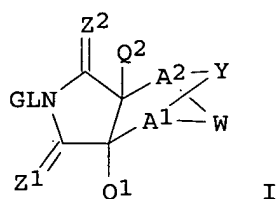
US 2001-25116

A 20011219

OTHER SOURCE(S):

MARPAT 139:164784

GI



AB Title compds. [I; G = (substituted) aryl, heterocyclyl; Z1, Z2 = O, S, NH, NR6; A1, A2 = CR7, N; Y = JJ'J"; J, J' = (CR7R7')n; n = 0-3, J' = bond, O, S, SO, SO2, NH, NR7, CR7R7', R2PO, R2PS, R2OPO, R2NHPO, OPOOR2, OPONHR2, OSO2, NHNH, NHNR6, NR6NH, N:N, (substituted) cycloalk(en)yl, heterocyclo; W' = CR7R7'CR7R7, CR7R7'CO, COCO, CR7R7'C:CH2, C:CH2C:CH2, CR7R7C:NR1, C:NR1C:NR1, NR9CR7R7, N:N, (substituted) cycloalk(en)yl, heterocyclo, aryl, etc.; Q1, Q2 = H, (substituted) alkyl, alkenyl, cycloalk(en)yl, heterocycloalkyl, aryl(alkyl), alkynyl, heterocyclo, halo, CN, R1O2C, R4CO, R5R6NCO, HOCR7R7', NO2, R1OCH2, R1O, NH2, COSR1, SO2R1, NR4R5; L = bond, (CR7R7')n, NH, NR5, NH(CR7R7')n, NR5(CR7R7')n; R1, R1' = H, R2; R2 = (substituted) alkyl, alkenyl, alkynyl, cycloalk(en)yl, heterocyclo, cycloalk(en)ylalkyl, heterocycloalkyl, aryl(alkyl); R3, R3' = R1, halo, CN, hydroxylamine, hydroxamide, (substituted) alkoxy, alkylthio, amino, NR1R2, SH; R4 = R1, R1CO, R1O2C, R1NHCO, SO2OR1, SO2R1, SO2NR1R1'; R5 = R2, R1CO, R1NHCO, SO2R1, SO2OR1, SO2NR1R1'; R6 = R5, CN, OH, OR1; R7, R7' = R4, halo, CN, OR4, NO2, hydroxylamine, hydroxylamide, amino, NHR4, NR2R5, NR5R5, NOR1, SH, (substituted) alkylthio, HO2C, R1CO2, NH2CO, SOR1, PO3R1R1', R1R1'NCO, COSR1; with provisos], were prepared as modulators of nuclear hormone receptor function (no data). Thus, 4-(tert-butyltrimethylsiloxy)-2H-thiopyran (preparation given) and 1-(4-bromo-3-methylphenyl)-1H-pyrrole-2,5-dione (preparation given) were refluxed 5 h in PhMe to give an enol ether intermediate which was stirred with CF3CO2H in CH2Cl2 to give 22% (3 α ,4 α ,7 α ,7 α)-2-(4-bromo-3-methylphenyl)tetrahydro-4,7-ethanothiopyrano[3,4-c]pyrrole-1,3,8(2H,4H)-trione.

IC ICM C07D491-00

ICS A61K031-40

CC 28-2 (Heterocyclic Compounds (More Than One Hetero Atom))

Section cross-reference(s): 1

IT	573722-37-9P	573722-38-0P	573722-39-1P	573722-40-4P	573722-41-5P
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Ward PCT/US03/21394

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573735-01-0P	573735-10-1P	573735-14-5P	573735-19-0P	573735-41-8P
573735-49-6P	573735-54-3P	573735-60-1P	573735-66-7P	573735-72-5P
573735-79-2P	573735-85-0P	573735-91-8P	573735-98-5P	573736-04-6P
573736-08-0P	573736-13-7P	573736-20-6P	573736-27-3P	573736-31-9P
573736-39-7P	573736-44-4P	573736-51-3P	573736-58-0P	573736-63-7P
573736-70-6P				

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); **BIOL (Biological study)**; PREP (Preparation);
 USES (Uses)

(preparation of fused succinimides as **modulators** of nuclear hormone receptor function)

IT **573730-33-3P**

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); **BIOL (Biological study)**; PREP (Preparation);
 USES (Uses)

(preparation of fused succinimides as **modulators** of nuclear hormone receptor function)

RN 573730-33-3 HCAPLUS

CN 1-Naphthalenecarbonitrile, 4-[(3aS,4R,7R,7aR)-octahydro-4-methyl-7-[2-[(5-methyl[1,2,4]triazolo[1,5-a]pyrimidin-7-yl)oxy]ethyl]-1,3-dioxo-4,7-epoxy-2H-isindol-2-yl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

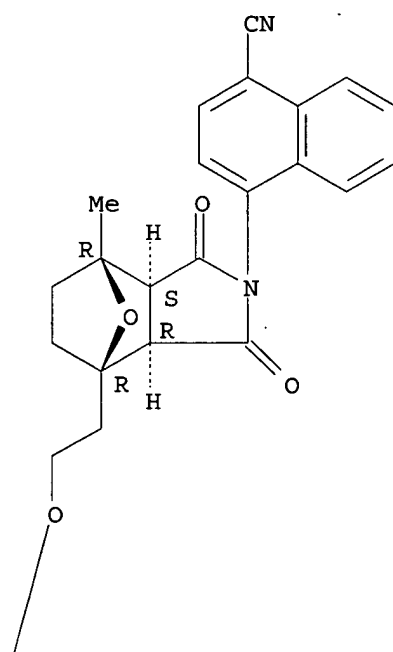
CM 1

CRN 573730-32-2

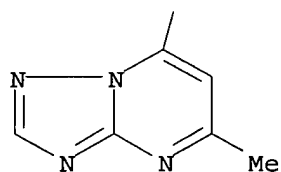
CMF C28 H24 N6 O4

Absolute stereochemistry.

PAGE 1-A



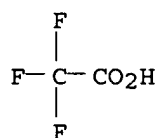
PAGE 2-A



CM 2

CRN 76-05-1

CMF C2 H F3 O2



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 5 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 2002:869496 HCAPLUS
 DOCUMENT NUMBER: 137:363033
 TITLE: Peptidomimetic modulators of cell adhesion
 INVENTOR(S): Gour, Barbara J.; Blaschuk, Orest W.; Ali, Anmar; Ni, Feng; Chen, Zhigang; Michaud, Stephanie D.; Wang, Shoameng; Hu, Zenzian
 PATENT ASSIGNEE(S): Can.
 SOURCE: U.S. Pat. Appl. Publ., 309 pp., Cont.-in-part of U.S. Ser. No. 491,078.
 CODEN: USXXCO
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 14
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2002168761	A1	20021114	US 2001-769145	20010124
US 2004006011	A1	20040108	US 2003-425557	20030428
PRIORITY APPLN. INFO.:			US 2000-491078	A2 20000124
			US 1996-21612P	P 19960712
			US 1997-893534	A1 19970711
			US 2000-507102	A1 20000217
			US 2001-769145	B2 20010124
			US 2001-6982	A2 20011204

OTHER SOURCE(S): MARPAT 137:363033

AB Peptidomimetics of cyclic peptides, and compns. comprising such peptidomimetics are provided. The peptidomimetics have a three-dimensional structure that is substantially similar to a three-dimensional structure of a cyclic peptide that comprises a cadherin cell adhesion recognition sequence HAV. Methods for using such peptidomimetics for modulating cadherin-mediated cell adhesion in a variety of contexts are also provided.

IC ICM A61K038-17
 ICS C07K014-435; C12N005-02

NCL 435325000

CC 1-3 (Pharmacology)

Section cross-reference(s): 34, 63

IT 57-88-5D, Cholest-5-en-3-ol (3 β)-, glycoside derivs. 135-16-0,
 L-Glutamic acid, N-[4-[(2-amino-1,4,5,6,7,8-hexahydro-4-oxo-6-pteridinyl)methyl]amino]benzoyl]- 487-49-0, Ethanone,
 1-(2,4-dihydroxyphenyl)-2-(4-methoxyphenyl)- 548-73-2,
 2H-Benzimidazol-2-one, 1-[1-[4-(4-fluorophenyl)-4-oxobutyl]-1,2,3,6-tetrahydro-4-pyridinyl]-1,3-dihydro- 570-88-7, Cholest-4-ene-3,6-diol, (3 β ,6 β)- 1210-66-8, 1H-Purin-6-amine, N-phenyl- 1482-74-2,
 2-Propen-1-one, 3-phenyl-1-(2,3,4-trihydroxyphenyl)- 1699-40-7,
 Benzeneacetamide, 4-methoxy-N-[2-[3-methoxy-4-(phenylmethoxy)phenyl]ethyl]-3-(phenylmethoxy)- 1776-30-3, 2-Propen-1-one, 1-(2,4-dihydroxyphenyl)-3-phenyl- 2486-02-4, Benzoic acid, 3,4,5-trihydroxy-, 3-methylbutyl ester 2810-37-9, 1H-Isoindole-1,3(2H)-dione, 2-[5-(1H-benzotriazol-1-yl)propyl]- 2979-51-3, 1H-Imidazole, 1-(1-oxo-3-phenyl-2-propenyl)- 3242-68-0,
 L-Glutamic acid, N-[4-[[2-[(2-amino-1,4-dihydro-4-oxo-5-pyrimidinyl)amino]ethyl]amino]benzoyl]- 3257-73-6, 9H-Purin-6-amine, 9-[2,3,5-tris-O-(phenylmethyl)- β -D-arabinofuranosyl]- 3561-56-6,
 L-Asparagine, N2-[(phenylmethoxy)carbonyl]-, (4-nitrophenyl)methyl ester

3566-25-4, L-Glutamic acid, N-[4-[[2-(2-amino-1,4-dihydro-4-oxo-6-pteridinyl)ethyl]amino]benzoyl]- 3575-07-3, 1H-Benzimidazole, 2,2'-(1,2-ethanediyl)bis- 3922-47-2, 1H-1,2,4-Triazol-3-amine, 5-[(phenylmethyl)thio]- 4672-96-2, Benzeneacetamide, 3-methoxy-N-[2-[4-methoxy-3-(phenylmethoxy)phenyl]ethyl]-4-(phenylmethoxy)- 5226-71-1, Benzene, 1,1'-[1,10-decanediylbis(oxy)]bis[3-nitro- 5341-00-4, 1,4-Naphthalenedione, 2-[3-(decahydro-2-naphthalenyl)propyl]-3-hydroxy- 5415-88-3, 1H-Purine-2,6-dione, 3,7-dihydro-1,3,7-trimethyl-8-(4-phenylbutoxy)- 5421-95-4, Urea, (3-phenyl-1,2,4-oxadiazol-5-yl)- 5426-87-9, Benzamide, N-[(2,3,6,7-tetrahydro-1,3-dimethyl-2,6-dioxo-1H-purin-8-yl)methyl]- 5429-46-9, Benzamide, N-[2-(2,3,6,7-tetrahydro-1,3-dimethyl-2,6-dioxo-1H-purin-8-yl)ethyl]- 5446-36-6, 1H-Purin-6-amine, N-(4-methylphenyl)- 5454-50-2, Ethanone, 1-phenyl-2-(1H-purin-6-ylthio)- 5454-52-4, 1H-Purine, 6-[(2-phenoxyethyl)thio]- 5508-58-7, 2(3H)-Furanone, 3-[2-[(1R,4aS,5R,6R,8aS)-decahydro-6-hydroxy-5-(hydroxymethyl)-5,8a-dimethyl-2-methylene-1-naphthalenyl]ethylidene]dihydro-4-hydroxy-, (3E,4S)- 5534-95-2 5800-34-0, Pentanoic acid, 5-[[[(1S)-2-[(4-nitrophenyl)amino]-2-oxo-1-(phenylmethyl)ethyl]amino]-5-oxo- 6286-57-3, 5(4H)-Isoxazolone, 4-(1,3-benzodioxol-5-ylmethylene)-3-phenyl- 6295-27-8, 7H-1,2,3-Triazolo[4,5-d]pyrimidin-7-one, 5-amino-2,6-dihydro-2-phenyl- 6300-80-7, Benzaldehyde, 4-(dimethylamino)-, 7H-purin-6-ylhydrazone 6320-71-4, 1,4-Naphthalenedione, 2-(4-cyclohexylbutyl)-3-hydroxy- 6322-09-4, 2(1H)-Quinoxalinone, 3-[2-(2-chlorophenyl)ethenyl]-7-methyl- 6323-88-2, 2(1H)-Quinoxalinone, 3-[2-(3-nitrophenyl)ethenyl]- 6323-89-3, 2(1H)-Quinoxalinone, 3-(2-phenylethenyl)- 6331-03-9, Benzaldehyde, 4-nitro-, 7H-purin-6-ylhydrazone 6338-84-7, 1H-Purine-2,6-dione, 3,7-dihydro-1,3,7-trimethyl-8-(2-phenylethyl)- 6340-76-7, 2,4-Pyrimidinediamine, 6-chloro-N4-(3-methylphenyl)- 6633-66-5, 2,4,6-Pyrimidinetriamine, N4-(4-bromophenyl)- 6807-82-5, L-Glutamic acid, N-[4-[[2-(2-amino-1,4-dihydro-4-oxo-6-pteridinyl)methyl]amino]benzoyl]-L- α -glutamyl- 6962-62-5, 2-Propen-1-one, 3-(1,3-benzodioxol-5-yl)-1-(2,4-dihydroxyphenyl)- 6975-34-4, 1H-Purine, 6-[(3-phenyl-2-propenyl)thio]- 7781-29-5, 2,4-Pyrimidinediamine, 6-methyl-N4-phenyl- 10320-97-5, 1,2,3,4-Thiatriazol-5-amine, N-1-naphthalenyl- 13184-14-0, L-Lysine, L-lysyl-L-lysyl- 13351-10-5, 2-Propen-1-one, 1-(2,4-dihydroxyphenyl)-3-(4-methoxyphenyl)- 13745-20-5, 2-Propen-1-one, 1-(2,4-dihydroxyphenyl)-3-(4-hydroxyphenyl)- 15013-60-2, Cholest-4-ene-3,6-diol, (3 β ,6 α)- 15970-42-0, 1H-Imidazole-1,2-diamine, 4-(4-chlorophenyl)- 16856-21-6, L-Tryptophan, N-[N-[(phenylmethoxy)carbonyl]-L-phenylalanyl]-, methyl ester 16879-84-8, L-Threonine, N-[(phenylmethoxy)carbonyl]-, (4-nitrophenyl)methyl ester 17357-75-4, 1H-1,2,4-Triazole, 3-[[[(4-methoxyphenyl)methyl]thio]- 17430-65-8, L-Tryptophan, N-[(phenylmethoxy)carbonyl]-L-valyl-, methyl ester 17496-31-0, 1H-Imidazole, 4-[[[(phenylmethyl)thio]methyl]- 18100-11-3, 1,4-Naphthalenedione, 2-(3-cyclohexylbutyl)-3-hydroxy- 18100-12-4, 1,4-Naphthalenedione, 2-[3-(4-chlorophenyl)propyl]-3-hydroxy- 18211-37-5, 1,4-Naphthalenedione, 2-hydroxy-3-[3-(4-methylphenyl)propyl]- 19312-13-1, 2-Propen-1-one, 1-(2,5-dihydroxyphenyl)-3-phenyl- 19484-75-4D, 2H-1-Benzopyran-2-one, 3,4-dihydro-7-hydroxy-4-methyl-, furanoside derivative 19889-31-7, 1H-Imidazole-4-propanamide, α -amino-N-2-naphthalenyl- 20621-49-2, 2-Propen-1-one, 1-(2,6-dihydroxy-4-methoxyphenyl)-3-(4-methoxyphenyl)- 20711-05-1, L-Glutamic acid, N-[4-[[2-(2-amino-1,5,6,7-tetrahydro-4-hydroxy-6-pteridinyl)ethyl]amino]benzoyl]- 21108-76-9, Imidazo[2,1-b]thiazol-3(2H)-one, 5,6-dihydro-2-(3-phenyl-2-propenylidene)- 21658-45-7, Glycine, L-arginyl-L-prolyl-L-prolyl- 23567-67-1, Phenol, 4-(1,2,3,4-thiatriazol-5-ylamino)- 23815-88-5, 1-6-Bradykinin 24205-32-1, L-Glutamic acid,

N-[4-[[[(2,4-diamino-5-methyl-6-quinazolinyl)methyl]amino]benzoyl]-
 ,diethylester 24386-39-8, Urea, N-1-naphthalenyl-N'-2-pyrimidinyl-
 24829-12-7, Phenol, 2-[(1H-1,2,4-triazol-3-ylimino)methyl]- 26962-50-5,
 2-Propen-1-one, 1-(2,4-dihydroxyphenyl)-3-(2-hydroxyphenyl)- 27069-81-4,
 L-Glutamic acid, N-[4-[[[(2-amino-1,4-dihydro-4-oxo-6-
 quinazolinyl)methyl]amino]benzoyl]-, diethyl ester 27430-15-5,
 4,6(1H,5H)-Pyrimidinedione, 5-[[4-(dimethylamino)phenyl]methylene]dihydro-
 2-thioxo- 27430-17-7, 4,6(1H,5H)-Pyrimidinedione, dihydro-5-(3-phenyl-2-
 propenylidene)-2-thioxo- 28005-33-6, Benzene, 1,1'-methylenebis[4-[(4-
 nitrophenyl)thio]- 28246-23-3, Ethanone, 2-(1H-imidazol-2-ylthio)-1-
 phenyl- 28772-56-7, 2H-1-Benzopyran-2-one, 3-[3-(4'-bromo[1,1'-biphenyl]-
 4-yl)-3-hydroxy-1-phenylpropyl]-4-hydroxy- 29654-52-2, Benzene,
 1,1'-methylenebis[4-[(4-nitrophenyl)sulfonyl]- 30148-18-6, Methanone,
 (4-chlorophenyl)(1-methyl-1H-imidazol-2-yl)- 30216-31-0D, Benzoxazole,
 2-[2-(2-chlorophenyl)ethenyl]-, derivs. 30355-60-3, 1,3,5-Triazine-2,4-
 diamine, 6-(chloromethyl)-N-phenyl- 30826-46-1, L-Glutamic acid,
 N-[4-[[[5,7-bis(acetylamino)pyrido[3,4-b]pyrazin-3-
 yl]methyl]methylamino]benzoyl]-, diethyl ester 30826-47-2, L-Glutamic
 acid, N-[4-[[[6,8-bis(acetylamino)pyrido[2,3-b]pyrazin-2-
 yl]methyl]methylamino]benzoyl]-, diethyl ester 33254-46-5,
 6H-Purine-6-thione, 1,9-dihydro-9-(3-phenylpropyl)- 34396-76-4,
 6H-Purin-6-one, 1,9-dihydro-9-(3-phenylpropyl)- 37664-31-6, Ethanone,
 1-(4-chlorophenyl)-2-(1H-1,2,4-triazol-3-ylthio)- 40538-65-6,
 5(4H)-Isoxazolone, 3-methyl-4-[(phenylamino)methylene]- 40816-36-2,
 4,6-Pyrimidinediamine, 5-nitro-N-phenyl- 41266-78-8,
 1H-1,2,4-Triazol-3-amine, 5-[[[(4-chlorophenyl)methyl]thio]- 41600-13-9,
 L-Glutamic acid, N-[4-[[[(2,4-diamino-6-pteridiny]methyl]methylamino]benzo
 yl]-L-γ-glutamyl- 42220-83-7, 2-Propen-1-one, 1-(2,4-
 dihydroxyphenyl)-3-(3-hydroxyphenyl)- 46825-86-9, Pyrimidinetetramine,
 N4-(4-bromophenyl)- 50602-77-2, L-Glutamic acid, N-[4-[[[(2,4-diamino-6-
 pteridiny]methyl]methylamino]benzoyl]-, dibutyl ester 51646-15-2***,
 [1,2,4]Triazolo[1,5-a]pyrimidine, 5,7-dimethyl-2-[(phenylmethyl)thio]-
 51893-98-2, Benzoic acid, 2-hydroxy-, [2-[(5-ethyl-1,4-dihydro-6-methyl-4-
 oxo-2-pyrimidinyl)thio]-1-phenylethylidene]hydrazide 51934-26-0,
 L-Glutamic acid, N-[4-[[[(7-amino-1,5-dihydro-5-thioxopyrimido[5,4-e]-1,2,4-
 triazin-3-yl)methyl]amino]benzoyl]-, diethyl ester, monohydrochloride
 51934-28-2, L-Glutamic acid, N-[4-[[[(5,7-diaminopyrimido[5,4-e]-1,2,4-
 triazin-3-yl)methyl]amino]benzoyl]-, diethyl ester 54299-50-2,
 2-Propen-1-one, 1-(2,4-dihydroxy-3,6-dimethoxyphenyl)-3-phenyl-
 54395-52-7, 1H-Isoindole-1,3(2H)-dione, 5,5'-[(1-methylethylidene)bis(4,1-
 phenyleneoxy)]bis[2-methyl- 56025-86-6, 1H-Purine-2,6-dione,
 3,7-dihydro-3-methyl-7-(phenylmethyl)- 56307-99-4, Ethanone,
 1-(2,4-dihydroxyphenyl)-2-(phenylthio)- 57710-80-2, 1H-Benzotriazole-1-
 carboxylic acid, phenylmethyl ester 57808-66-9, 2H-Benzimidazol-2-one,
 5-chloro-1-[1-[3-(2,3-dihydro-2-oxo-1H-benzimidazol-1-yl)propyl]-4-
 piperidinyl]-1,3-dihydro- 57966-42-4, L-Threonine, L-arginyl-L-tyrosyl-L-
 leucyl-L-prolyl- 58677-09-1, L-Glutamic acid, N-[4-[[[(2-amino-1,4-
 dihydro-4-oxo-6-quinazolinyl)methyl]methylamino]benzoyl]-, diethyl ester
 60045-61-6, 4,6(1H,5H)-Pyrimidinedione, dihydro-5-[(4-
 methoxyphenyl)methylene]-2-thioxo- 60407-48-9, L-Isoleucine,
 L-arginylglycyl-L-prolyl-L-phenylalanyl-L-prolyl- 60482-96-4, L-Leucine,
 L-arginyl-L-prolyl-L-tyrosyl-L-isoleucyl- 61043-53-6,
 L-Phenylalaninamide, N-(3-carboxy-1-oxopropyl)-L-alanyl-L-alanyl-N-(4-
 nitrophenyl)- 64792-21-8, 2-Propenal, 3-phenyl-, (1,4-dihydro-6-methyl-4-
 oxo-2-pyrimidinyl)hydrazone 64801-58-7, L-Aspartic acid,
 N-[4-[[[(2,4-diamino-6-pteridiny]methyl]methylamino]benzoyl]-L-γ-
 glutamyl- 65147-09-3, L-Argininamide, N-[(1,1-dimethylethoxy)carbonyl]-L-
 leucylglycyl-N-(4-methyl-2-oxo-2H-1-benzopyran-7-yl)- 65757-04-2,
 L-Glutamic acid, N-[4-[[[(1,2,3,4-tetrahydro-2-imino-1,3-dimethyl-4-oxo-6-

pteridiny]methyl]amino]benzoyl]-, dimethyl ester 65757-05-3, L-Glutamic acid, N-[4-[[[(2-amino-3,4-dihydro-3-methyl-4-oxo-6-pteridiny]methyl]amino]benzoyl]-, dimethyl ester 65877-43-2D, 1,3-Benzenediol, 5-[2-(3-hydroxy-4-methoxyphenyl)ethenyl]-, glycoside derivative 66048-53-1, Guanosine, 2',3',5'-tribenzoate 66147-31-7, L-Glutamic acid, N-[4-[[[(2,4-diamino-6-pteridiny]methyl]methylamino]benzoyl]-, 5-butyl ester 67368-29-0, L-Alanine, L-methionyl-L-arginyl-L-phenylalanyl- 67655-19-0, Phenol, 2,2'-[(2-hydroxy-1,3-propanediyl)bis(oxy)]bis- 67836-16-2, Acetamide, 2-(2,4-dichlorophenoxy)-N-1H-1,2,4-triazol-3-yl- 68047-41-6, 1,3,4-Oxadiazole, 2-(3-bromophenyl)-5-(2-naphthalenyl)- 68215-68-9, Phenol, 2-[4-amino-6-[(4-chlorophenyl)amino]-1,3,5-triazin-2-yl]-4-chloro-68682-02-0, 4H-1-Benzopyran-4-one, 2,3-dihydro-5,7-dihydroxy-2-(4-hydroxyphenyl)-8-(3-methyl-2-butenyl)- 68838-40-4, 1H-1,2,4-Triazole, 3-methyl-5-[(phenylmethyl)thio]- 69097-98-9, 4H-1-Benzopyran-4-one, 2,3-dihydro-5,7-dihydroxy-2-(4-hydroxy-3-methoxyphenyl)- 69193-20-0, 4-Pyrimidinamine, 5-bromo-N-phenyl- 69480-15-5, 3H-1,2,4-Triazole-3-thione, 5-[4-(1,1-dimethylethyl)phenyl]-1,2-dihydro- 70280-72-7, L-Glutamic acid, N-[4-[[[(2,4-diamino-6-pteridiny]methyl] (phenylmethyl) amino]benzoyl]-, diethyl ester 70280-75-0, L-Glutamic acid, N-[4-[[[(2,4-diamino-6-pteridiny]methyl]ethylamino]benzoyl]-, diethyl ester 70539-54-7, L-Glutamic acid, N-[3,5-dichloro-4-[[[(2,4-diamino-6-pteridiny]methyl]ethylamino]benzoyl]-, diethyl ester 70968-04-6, L-Leucinamide, N-(3-carboxy-1-oxopropyl)-L-alanyl-L-alanyl-L-prolyl-N-(4-nitrophenyl)- 71047-38-6, 1H-Imidazole, 1-(3,7-dimethyl-2,6-octadienyl)-71074-46-9, Glycine, N-[N-[4-[[[(2,4-diamino-6-pteridiny]methyl]methylamino]benzoyl]-L-γ-glutamyl]- 71074-48-1, L-Aspartic acid, N-[4-[[[(2,4-diamino-6-pteridiny]methyl]methylamino]benzoyl]-L-α-glutamyl- 71074-49-2, L-Glutamic acid, N-[4-[[[(2,4-diamino-6-pteridiny]methyl]methylamino]benzoyl]-L-α-glutamyl- 71707-02-3, L-Glutamic acid, N-[N-[4-[[[(2,4-diamino-6-pteridiny]methyl]amino]benzoyl]-L-γ-glutamyl]- 72630-15-0, Glutamic acid, N-[4-[[2-(2-amino-1,4,5,6,7,8-hexahydro-5-methyl-4-oxo-6-pteridiny]ethyl]amino]benzoyl]- 72682-77-0, L-Isoleucinamide, N-(3-carboxy-1-oxopropyl)-L-alanyl-L-alanyl-L-prolyl-N-(4-nitrophenyl)-72704-76-8, 2-Propen-1-one, 3-(3,4-dihydroxyphenyl)-1-phenyl-73554-90-2, L-Argininamide, N-[(1,1-dimethylethoxy)carbonyl]-L-phenylalanyl-L-seryl-N-(4-methyl-2-oxo-2H-1-benzopyran-7-yl)-73572-58-4, L-Phenylalanine, N-[(1,1-dimethylethoxy)carbonyl]-L-phenylalanyl-L-leucyl-L-phenylalanyl-L-leucyl- 74039-67-1, 1H-Purine-2,6-dione, 3,7-dihydro-1,3-dimethyl-8-(3-phenyl-2-propenyl)-74405-42-8, Adenosine, N-benzoyl-5'-O-[bis(4-methoxyphenyl)phenylmethyl]-2'-deoxy-, 3'-(hydrogen butanedioate) 74405-44-0, Cytidine, N-benzoyl-5'-O-[bis(4-methoxyphenyl)phenylmethyl]-2'-deoxy-, 3'-(hydrogen butanedioate) 74853-69-3, L-Leucine, N2-acetyl-L-arginyl-L-arginyl-L-prolyl-L-tyrosyl-L-isoleucyl- 75651-68-2, L-Phenylalaninamide, N-(3-carboxy-1-oxopropyl)-L-phenylalanyl-L-prolyl-N-(4-nitrophenyl)-75960-43-9, 1H-Imidazole-4-hexanoic acid, 5-(chloromethyl)-2,3-dihydro-ε,2-dioxo-, ethyl ester 76172-68-4, 1-Propanone, 3-(4-methoxyphenyl)-1-(2,4,6-trihydroxyphenyl)- 80032-99-1, 1H-1,2,4-Triazole, 3,3'-[1,4-butanediylbis(thio)]bis- 80360-08-3, L-Glutamic acid, N-[4-[[[(2,4-diaminopyrido[2,3-d]pyrimidin-6-yl)methyl]amino]benzoyl]-, diethyl ester 81066-61-7, 2-Pyridinamine, 3-[[4-(1,1-dimethylethyl)phenyl]methoxy]- 81587-37-3, 3-Pyridinethiol, 2-[(2,6-diamino-4-pyrimidinyl)amino]-6-methyl- 82628-82-8, 1-Propanone, 3-(4-nitrophenyl)-1-(2,4,6-trihydroxyphenyl)- 82855-85-4, L-Glutamic acid, N-[4-[[[(2-amino-1,4,5,6,7,8-hexahydro-4-oxopyrido[3,2-d]pyrimidin-6-yl)methyl]amino]benzoyl]-, diethyl ester 85122-85-6, 1H-Isoindole-1,3(2H)-dione, 2,2'-[1,3-propanediylbis(4,1-

piperidinediylmethylene)]bis- 86669-33-2, L-Glutamic acid,
 N-[4-[[[(2,4-diamino-6-pteridiny]methyl)methylamino]benzoyl]-,
 bis(1,1-dimethylethyl) ester 90259-60-2, Benzamide, 2-amino-N-[3-(1H-
 imidazol-1-yl)propyl]- 90259-61-3, Benzamide, 2-[[[(4-
 chlorophenyl)sulfonyl]amino]-N-[3-(1H-imidazol-1-yl)propyl]- 92899-39-3,
 Glycine, L-valylglycyl-L-valyl-L-alanyl-L-prolyl- 92954-99-9, Glycine,
 1-acetyl-L-prolyl-L-leucylglycyl-L-leucyl-L-leucyl-, ethyl ester
 93515-01-6, L-Threonine, L-tyrosyl-L-prolyl-L-prolyl-L- α -glutamyl-L-
 prolyl-L- α -glutamyl- 93524-30-2, β -D-Glucopyranosiduronic
 acid, (3 α ,5 β)-21-(acetyloxy)-20-[(aminocarbonyl)hydrazono]pregn
 an-3-yl, methyl ester, 2,3,4-triacetate 93674-97-6, L-Serine,
 L-arginylglycyl-L- α -glutamyl- 95192-21-5, L-Phenylalaninamide,
 N-(3-carboxy-1-oxopropyl)-L-phenylalanyl-L-alanyl-N-(4-nitrophenyl)-
 95192-38-4, L-Phenylalaninamide, N-(3-carboxy-1-oxopropyl)-L-alanyl-L-
 valyl-L-prolyl-N-(4-nitrophenyl)- 95210-75-6, L-Proline,
 L-tyrosyl-L-prolyl-L-phenylalanyl-L-valyl-L- α -glutamyl-L-prolyl-L-
 isoleucyl- 98018-39-4, Ethanone, 2-[(2-amino-1H-purin-6-yl)thio]-1-
 phenyl- 98151-93-0, L-Proline, L-tyrosyl-L-prolyl-L-phenylalanyl-L-
 prolylglycyl-L-prolyl-L-isoleucyl- 100975-56-2, Benzaldehyde,
 4-hydroxy-, (2,3,6,7-tetrahydro-1,3,7-trimethyl-2,6-dioxo-1H-purin-8-
 yl)hydrazone 102212-40-8, 1H-Purine-2,6-dione, 3,7-dihydro-1,3-dimethyl-
 8-[(2-phenylethyl)amino]- 103030-49-5, 2,4-Pyrimidinediamine,
 N4-(4-chlorophenyl)-5-nitro- 103398-43-2, Benzenemethanol,
 2-[bis[2-[(4-nitrobenzoyl)oxy]ethyl]amino]-, 4-nitrobenzoate (ester)
 105037-36-3, Benzenesulfonic acid, 4-[(7-chloro-4-quinazolinyl)amino]-
 108608-63-5, Glycine, L-seryl-L- α -aspartylglycyl-L-arginyl-
 110906-89-3, L-Phenylalaninamide, N-(3-carboxy-1-oxopropyl)-L-phenylalanyl-
 L-alanyl-L-alanyl-N-(4-nitrophenyl)- 111172-14-6, 1,3-Benzodioxole-5-
 carboxaldehyde, O-(2-thienylcarbonyl)oxime 112233-74-6, Carbamic acid,
 diphenyl-, 2-(acetyl-amino)-1H-purin-6-yl ester 113866-00-5,
 L-Argininamide, N-[(1,1-dimethylethoxy)carbonyl]-L- α -aspartyl-L-
 prolyl-N-(4-methyl-2-oxo-2H-1-benzopyran-7-yl)-, phenylmethyl ester
 113866-16-3, L-Argininamide, N-[(1,1-dimethylethoxy)carbonyl]-L- α -
 glutamyl-L-alanyl-N-(4-methyl-2-oxo-2H-1-benzopyran-7-yl)-, phenylmethyl
 ester 117889-48-2, 1H-Tetrazole, 5-[(2,4-dichlorophenoxy)methyl]-
 118034-92-7, L-Threonine, L-histidyl-L-phenylalanyl-L-methionyl-L-prolyl-
 120225-54-9, Benzenepropanoic acid, 4-[2-[[[6-amino-9-(N-ethyl- β -D-
 ribofuranuronamidosyl)-9H-purin-2-yl]amino]ethyl]- 121036-80-4,
 1,2,4-Triazin-5(2H)-one, 6-[2-(4-methylphenyl)ethenyl]-3-phenyl-
 121036-81-5, 1,2,4-Triazin-5(2H)-one, 6-[2-(4-methoxyphenyl)ethenyl]-3-
 phenyl- 124485-41-2, L-Argininamide, N-[(phenylmethoxy)carbonyl]-L-valyl-
 L-valyl-N-(4-methyl-2-oxo-2H-1-benzopyran-7-yl)- 126235-09-4,
 1H-Purine-2,6-dione, 3,7-dihydro-1,3-dimethyl-8-(2-phenylethyl)-
 128802-79-9, L-Phenylalaninamide, N-(3-carboxy-1-oxopropyl)-L-alanyl-L-
 isoleucyl-L-prolyl-N-(4-nitrophenyl)- 131061-65-9, 7H-Purine-7-butanolic
 acid, 1,2,3,6-tetrahydro-1,3-dimethyl-2,6-dioxo-8-[(phenylmethyl)amino]-,
 ethyl ester 132467-01-7, 2(1H)-Quinoxalinone, 3-[2-(2-
 chlorophenyl)ethenyl]- 133061-57-1, 2,4-Pyrimidinediamine,
 N4-(3,5-dichlorophenyl)-6-methyl- 134759-22-1, 1H-Thieno[3,4-d]imidazole-
 4-pentanamide, N-[6-[[[5-[[[(3',6'-dihydroxy-3-oxospiro[isobenzofuran-
 1(3H),9'-[9H]xanthen)-5-yl]amino]thioxomethyl]amino]pentyl]amino]-6-
 oxohexyl]hexahydro-2-oxo-, (3aS,4S,6aR)- 134796-34-2, 1H-1,2,4-Triazole,
 3-[[[(4-chlorophenyl)methyl]thio]- 137484-84-5, 1,3,5-Triazin-2-amine,
 4-chloro-6-[3-(2-furanyl)propoxy]-N,N-dimethyl- 137833-31-9,
 Myelo peptide 2 138194-56-6, 1H-Pyrrole-2,5-dione, 1-[3-[[[(4-oxo-1,2,3-
 benzotriazin-3(4H)-yl)oxy]carbonyl]phenyl]- 138915-75-0, L-Leucine,
 N-acetyl-L-histidyl-L-tryptophyl-L-alanyl-L-valylglycyl-L-histidyl-
 142206-40-4
 , 1H-Benzimidazole, 2,2'-(1,3-propanediyl)bis[1-methyl- 143113-41-1,

L-Valine, L-Histidyl-L-Alanyl 146871-70-7, 4-Quinazolinamine, N-(3-chlorophenyl)-, monohydrochloride 148337-06-8, Glycine, L-prolylglycyl-L-alanyl-L-isoleucyl-L-prolyl- 151358-70-2, 2-Propen-1-one, 1,1'-(2,6-pyridinediyl)bis[3-(4-hydroxyphenyl)- 152028-96-1, 1H-Imidazole, 4-[3-[(4-iodophenyl)methoxy]propyl]- 154719-25-2, L-Lysinamide, N-acetyl-L-tyrosyl-L-valyl-N-[(1S)-1-(carboxymethyl)-3-[(2,6-dimethylbenzoyl)oxy]-2-oxopropyl]-N6-[5-[(3aS,4S,6aR)-hexahydro-2-oxo-1H-thieno[3,4-d]imidazol-4-yl]-1-oxopentyl]- 155373-59-4, 4H-1-Benzopyran-4-one, 3-[[4-(1H-tetrazol-5-yl)phenyl]methyl]- 155373-72-1, 4H-1-Benzopyran-4-one, 2-phenyl-7-[4-(1H-tetrazol-5-yl)butoxy]- 160347-57-9D, 2(1H)-Pyrimidinone, 5-(4-pentylphenyl)-, derivs. 185503-97-3, L-Lysine, N6-[[4-[[4-(dimethylamino)phenyl]azo]phenyl]sulfonyl]-N2-[(9H-fluoren-9-ylmethoxy)carbonyl]- 188966-22-5D, Phenol, 2-(2H-benzotriazol-2-yl)-4-(1,1-dimethylhexyl)-, derivs. 191411-47-9, 1H-Imidazole-5-methanol, 1-methyl-2-[(phenylmethyl)thio]- 194424-08-3, Glutamic acid, N-[4-[[3-(2-thienyl)-2-quinoxaliny]amino]benzoyl]-, dipropyl ester 195140-70-6, 1H-Imidazole, 1-[2-(phenylmethoxy)ethyl]- 196600-87-0, Tyrosine, N-[(phenylmethoxy)carbonyl]norvalylglycyl-, methyl ester 197456-56-7, 1,4-Naphthalenedione, 2-[4-(decahydro-2-naphthalenyl)butyl]-3-hydroxy- 198488-04-9, Urea, N,N'-(3,3'-dimethyl[1,1'-biphenyl]-4,4'-diyl)bis[N'-(2-methylphenyl)- 198632-08-5, L-Proline, glycyl-L-arginylglycyl-L- α -glutamyl-L-threonyl- 199929-21-0, 1,4-Naphthalenedione, 2-hydroxy-3-[8-(4-methylphenoxy)octyl]- 200058-34-0, 1,4-Naphthalenedione, 2-(3-[1,1'-bicyclohexyl]-4-ylpropyl)-3-hydroxy- 200061-22-9, Phenol, 4,4'-(1-methylethylidene)bis-, bis(3,5-dinitrobenzoate) 200431-98-7, 3-Pyridinemethanamine, N-1H-1,2,4-triazol-3-yl- 200505-51-7, Decanedioic acid, bis[[4-(ethoxy-3-methoxyphenyl)methylene]hydrazide] 200706-30-5, 4H-1,2,4-Triazol-4-amine, N-[(2,3-dihydro-1H-inden-5-yl)methylene]- 200706-45-2, 4-Imidazolidinone, 5-[(2,3-dihydro-1H-inden-5-yl)methylene]-2-thioxo- 201997-13-9, 1,3-Benzenediol, 4-[[[2-hydroxy-2-(4-nitrophenyl)ethyl]imino]methyl]- 202118-27-2, 1H-1,2,4-Triazol-3-amine, N-[(2-iodophenyl)methylene]- 202118-28-3, 1H-1,2,4-Triazol-3-amine, N-[(2-chlorophenyl)methylene]- 202332-09-0, 1,4-Benzenediol, 2-(6-methylheptyl)- 202528-15-2, Cyclo(L-alanyl-L-histidyl-L-alanyl-L-valyl-L- α -aspartyl-L-isoleucyl) 206360-24-9, 4H-1-Benzopyran-4-one, 2,3-dihydro-5,7-dihydroxy-2-(4-hydroxyphenyl)-3-(3-methyl-2-butenyl)- 210709-22-1, L-Alanine, N2-benzoyl-L-arginyl-L-phenylalanyl- 215434-58-5, 1-Piperazinecarbothioamide, N-3-pyridinyl-4-[4-(trifluoromethyl)-2-pyrimidinyl]- 215655-36-0, Benzoic acid, 2-[[[2-[[4-(trifluoromethyl)-2-pyrimidinyl]amino]ethyl]amino]carbonyl]- 215657-86-6, 2-Pyrrolidinone, 1-[2-hydroxy-3-[4-[4-(trifluoromethyl)-2-pyrimidinyl]-1-piperazinyl]propyl]- 216299-43-3, 2,5-Pyrrolidinedione, 1-[[11-[(5-azido-1-naphthalenyl)oxy]-1-oxoundecyl]oxy]-
 RL: BSU (Biological study, unclassified); PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); ***BIOL (Biological study); USES (Uses)

(peptidomimetic modulators of cadherin-mediated cell adhesion for therapeutic use in relation to three-dimensional structure)

IT 51646-15-2, [1,2,4]Triazolo[1,5-a]pyrimidine, 5,7-dimethyl-2-[(phenylmethyl)thio]-

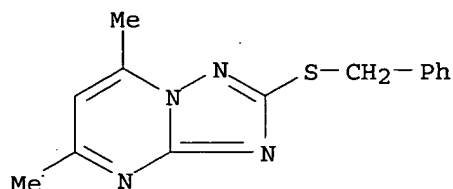
RL: BSU (Biological study, unclassified); PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(peptidomimetic modulators of cadherin-mediated cell adhesion for therapeutic use in relation to three-dimensional structure)

RN 51646-15-2 HCAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidine, 5,7-dimethyl-2-[(phenylmethyl)thio]-

(9CI) (CA INDEX NAME)



L24 ANSWER 6 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2001:545724 HCAPLUS

DOCUMENT NUMBER: 135:147398

TITLE: Peptidomimetic modulators of cell adhesion

INVENTOR(S): Gour, Barbara J.; Blaschuk, Orest W.; Ali, Anmar; Ni, Feng; Chen, Zhigang; Michaud, Stephanie Denise; Wang, Shoameng; Hu, Zengjian

PATENT ASSIGNEE(S): Adherex Technologies, Inc., Can.

SOURCE: PCT Int. Appl., 416 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 14

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001053331	A2	20010726	WO 2001-US2508	20010124
WO 2001053331	A3	20020711		
WO 2001053331	C2	20021031		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 2000-491078 A 20000124

OTHER SOURCE(S): MARPAT 135:147398

AB Peptidomimetics of cyclic peptides, and compns. comprising such peptidomimetics are provided. The peptidomimetics have a three-dimensional structure that is substantially similar to a three-dimensional structure of a cyclic peptide that comprises a cadherin cell adhesion recognition sequence HAV. Methods for using such peptidomimetics for modulating cadherin-mediated cell adhesion in a variety of contexts are also provided.

IC ICM C07K007-00

CC 1-3 (Pharmacology)

Section cross-reference(s): 34, 63

IT 57-88-5D, Cholest-5-en-3-ol (3 β)-, glycoside derivs. 135-16-0

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 134759-22-1 134796-34-2 137484-84-5 137833-31-9, Myelopeptide 2
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 151358-70-2 152028-96-1 154719-25-2 155373-59-4 155373-72-1
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 194424-08-3 195140-70-6 196600-87-0 197456-56-7 198488-04-9
 198632-08-5 199929-21-0 200058-34-0 200061-22-9 200431-98-7
 200505-51-7 200706-30-5 200706-45-2 201997-13-9 202118-27-2
 202118-28-3 202332-09-0 202528-15-2 206360-24-9 210709-22-1
 215434-58-5 215655-36-0 215657-86-6

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); PROC (Process); USES (Uses)

(peptidomimetic modulators of cell adhesion)

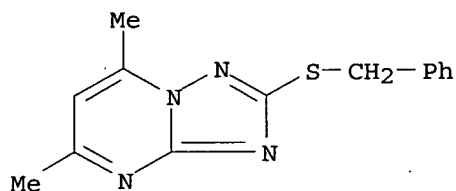
IT 51646-15-2

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); PROC (Process); USES (Uses)

(peptidomimetic modulators of cell adhesion)

RN 51646-15-2 HCAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidine, 5,7-dimethyl-2-[(phenylmethyl)thio]-(9CI) (CA INDEX NAME)



L24 ANSWER 7 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1998:402315 HCAPLUS

DOCUMENT NUMBER: 129:81753

TITLE: Preparation of substituted aryl piperazines as modulators of chemokine receptor activity

INVENTOR(S): Mills, Sander G.; Springer, Martin S.; MacCoss, Malcolm

PATENT ASSIGNEE(S): Merck & Co., Inc., USA; Mills, Sander G.; Springer, Martin S.; MacCoss, Malcolm

SOURCE: PCT Int. Appl., 185 pp.

CODEN: PIXXD2

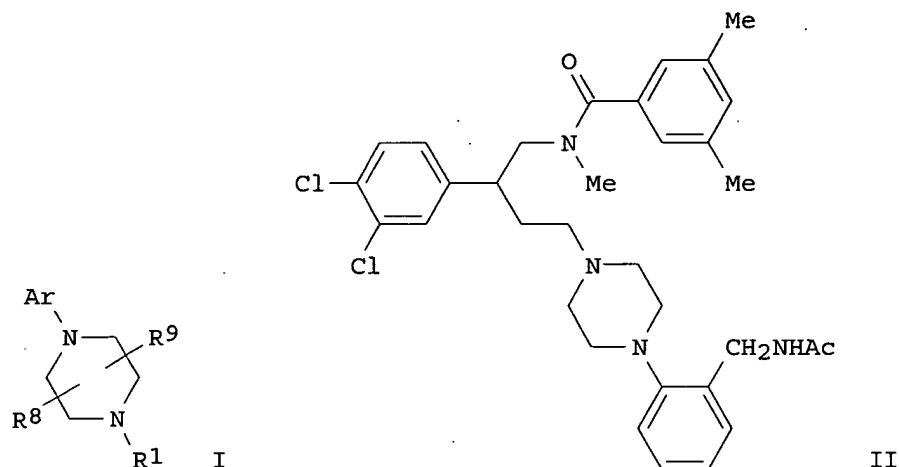
DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9825617	A1	19980618	WO 1997-US22769	19971212
W: AL, AM, AU, AZ, BA, BB, BG, BR, BY, CA, CN, CU, CZ, EE, GE, GW, HU, ID, IL, IS, JP, KG, KR, KZ, LC, LK, LR, LT, LV, MD, MG, MK, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, SL, TJ, TM, TR, TT, UA, US, UZ, VN, YU, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9855224	A1	19980703	AU 1998-55224	19971212
PRIORITY APPLN. INFO.:			US 1996-32889P	P 19961213
			US 1996-33567P	P 19961220
			WO 1997-US22769	W 19971212
OTHER SOURCE(S):			MARPAT 129:81753	
GI				



AB The title compds. [I; R¹ = (un)substituted C1-8 alkyl, C1-8 alkenyl; the nitrogen attached to R¹ is optionally quaternized with C1-4 alkyl or phenylC1-4alkyl or is optionally present as N-oxide; Ar = (un)substituted Ph, pyridyl, pyrimidyl, etc.; R⁸, R⁹ = H, (un)substituted C1-4 alkyl], useful as modulators of chemokine receptor activity, were prepared. Thus, 5-step synthesis of the title compound 3(S)-II starting from 3,5-dimethylbenzoic acid and 3(S)-(3,4-dichlorophenyl)-4-methylamino-1-pentene was described. In particular, compds. I are useful as modulators of the chemokine receptors CCR-1, CCR-2, CCR-2A, CCR-2B, CCR-3, CCR-4, CCR-5, CXCR-3, and/or CXCR-4. Compds. I can be used for preventing infection by HIV, treating infection by HIV, delaying of the onset of AIDS, or treating AIDS. Compds. I are effective at 0.1-5 mg/kg/day.

IC ICM A61K031-495

ICS A61K031-50

CC 28-17 (Heterocyclic Compounds (More Than One Hetero Atom))

Section cross-reference(s): 1

IT 179249-56-0P 179249-57-1P 179249-58-2P 179249-59-3P 179249-60-6P
 179249-61-7P 179249-62-8P 179249-63-9P 179249-64-0P 179249-65-1P
 179249-66-2P 179249-67-3P 179249-68-4P 179249-69-5P 179249-70-8P
 179249-71-9P 179249-72-0P 179249-73-1P 179249-74-2P 179249-75-3P
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 209160-62-3P 209160-63-4P 209160-64-5P 209160-65-6P 209160-66-7P
 209160-67-8P 209160-68-9P 209160-69-0P 209160-70-3P 209160-71-4P

209160-72-5P 209160-73-6P 209160-74-7P 209160-75-8P 209160-76-9P
209160-77-0P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of substituted aryl piperazines as modulators of chemokine receptor activity)

IT 92-54-6, 1-Phenylpiperazine 100-07-2, p-Anisoyl chloride 109-00-2, 3-Hydroxypyridine 142-08-5, 2(1H)-Pyridinone 288-32-4, Imidazole, reactions 288-88-0, 1H-1,2,4-Triazole 288-94-8, 1H-Tetrazole 394-47-8, o-Fluorobenzonitrile 446-52-6, 2-Fluorobenzaldehyde 499-06-9, 3,5-Dimethylbenzoic acid 725-89-3, 3,5-Bis(trifluoromethyl)benzoic acid 785-56-8, 3,5-Bis(trifluoromethyl)benzoyl chloride 1493-27-2, o-Fluoronitrobenzene 2905-62-6, 3,5-Dichlorobenzoyl chloride 13058-77-0, 8-Chloro-1,7-naphthyridine 39512-51-1, 1-(2-Methylphenyl)piperazine 52341-91-0 57260-71-6 72762-00-6, 2-Hydroxypyridine 74803-32-0 84400-99-7, 7-Chlorofuro[2,3-c]pyridine 90719-32-7, 4(S)-Benzyl-2-oxazolidinone 111896-72-1 121371-44-6 147643-57-0 156300-01-5 179250-63-6 179250-64-7 179250-65-8 179250-66-9 209160-84-9 209160-85-0 209160-86-1 209160-87-2 209160-88-3 209160-89-4 209160-90-7 209160-92-9 209160-93-0

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of substituted aryl piperazines as modulators of chemokine receptor activity)

IT 59084-06-9P 59215-38-2P 91646-29-6P 164328-62-5P 164329-19-5P 164329-21-9P 167483-86-5P 167484-59-5P 170017-73-9P 170017-74-0P 174855-53-9P 174855-57-3P 174855-59-5P 179250-25-0P 179250-27-2P 179250-28-3P 179250-29-4P 179250-30-7P 179250-31-8P 179250-32-9P 179250-33-0P 179250-34-1P 179250-35-2P 179250-36-3P 179250-37-4P 179250-38-5P 179250-39-6P 179250-40-9P 179250-41-0P 179250-42-1P 179250-43-2P 179250-44-3P 179250-45-4P 179250-46-5P 179250-47-6P 179250-48-7P 179250-49-8P 179250-50-1P 179250-51-2P 179250-52-3P 179250-53-4P 179250-54-5P 179250-55-6P 179250-56-7P 179250-58-9P 179250-59-0P 179250-60-3P 179250-61-4P 199105-20-9P 209160-78-1P 209160-79-2P 209160-80-5P 209160-81-6P 209160-82-7P 209160-91-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of substituted aryl piperazines as modulators of chemokine receptor activity)

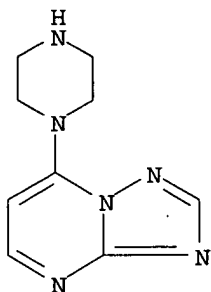
IT 179250-57-8P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of substituted aryl piperazines as modulators of chemokine receptor activity)

RN 179250-57-8 HCAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidine, 7-(1-piperazinyl)-, dihydrochloride (9CI) (CA INDEX NAME)



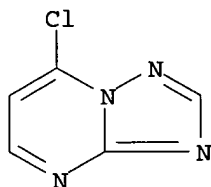
● 2 HCl

IT 52341-91-0

RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of substituted aryl piperazines as **modulators** of
chemokine receptor activity)

RN 52341-91-0 HCAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidine, 7-chloro- (9CI) (CA INDEX NAME)

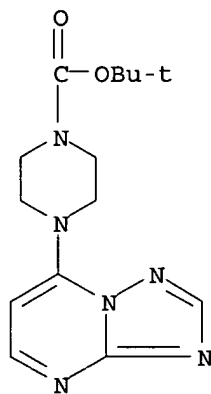


IT 179250-56-7P 179250-58-9P

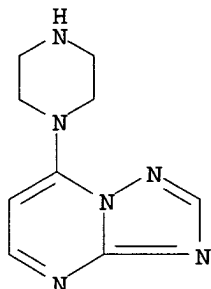
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(preparation of substituted aryl piperazines as **modulators** of
chemokine receptor activity)

RN 179250-56-7 HCAPLUS

CN 1-Piperazinecarboxylic acid, 4-[1,2,4]triazolo[1,5-a]pyrimidin-7-yl-,
1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



RN 179250-58-9 HCAPLUS
 CN [1,2,4]Triazolo[1,5-a]pyrimidine, 7-(1-piperazinyl)- (9CI) (CA INDEX NAME)

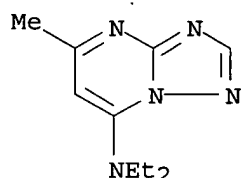


REFERENCE COUNT: 4. THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 8 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 1996:306356 HCAPLUS
 DOCUMENT NUMBER: 124:352464
 TITLE: Modulation of the dissolution profiles from Geomatrix multi-layer matrix tablets containing drugs of different solubility
 AUTHOR(S): Conte, U.; Maggi, L.
 CORPORATE SOURCE: Dep. Pharmaceutical Chem., Univ. Pavia, Pavia, I-27100, Italy
 SOURCE: Biomaterials (1996), 17(9), 889-896
 CODEN: BIMADU; ISSN: 0142-9612
 PUBLISHER: Elsevier
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB A new multi-layer tablet design consists in the application of a drug-free barrier layer on one or both bases of an active core (hydrophilic matrix). The partial coating modulates the core hydration process and reduces the surface area available for drug release. The result is an extended release that draws close to a linear profile. The device was mainly intended for soluble drugs, while an excessive reduction of the release rate may be obtained with drugs of low solubility. In this study a new time-dependent polymeric barrier is proposed to control the release of sparingly soluble drugs. Two different barrier compns. (one swellable and one erodible) are applied on active cores containing drugs of different water solubility, trapidil, ketoprofen and nicardipine-HCl, and the drug dissoln. patterns of the different multi-layer devices are compared. During dissoln., the swellable barrier swells and gels, but is not eroded, thus acting as a modulating membrane during the release process. The erodible barrier, instead, is progressively removed by the dissoln. medium, exposing in time an increasing extent of the planar surface(s) of the core to interaction with the outer environment and to drug release. Both types of coatings are able to control drug release from the devices: the swellable barrier shows a stronger modulation efficiency and is more suitable to modify the delivery pattern of highly soluble drugs; the erodible barrier shows a time-dependent coating effect that provides better control of the dissoln. profile of sparingly soluble drugs.

CC 63-5 (Pharmaceuticals)
 IT 15421-84-8, Trapidil 22071-15-4, Ketoprofen 54527-84-3,
 Nicardipine hydrochloride
 RL: PEP (Physical, engineering or chemical process); THU (Therapeutic
 use); BIOL (Biological study); PROC (Process); USES (Uses)
 (modulation of dissoln. profiles from Geomatrix multi-layer
 matrix tablets)
 IT 15421-84-8, Trapidil
 RL: PEP (Physical, engineering or chemical process); THU (Therapeutic
 use); BIOL (Biological study); PROC (Process); USES (Uses)
 (modulation of dissoln. profiles from Geomatrix multi-layer
 matrix tablets)
 RN 15421-84-8 HCAPLUS
 CN [1,2,4]Triazolo[1,5-a]pyrimidin-7-amine, N,N-diethyl-5-methyl- (9CI) (CA
 INDEX NAME)



L24 ANSWER 9 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1995:701937 HCAPLUS

DOCUMENT NUMBER: 123:313997

TITLE: Preparation of 7-phenoxyalkyl-1,2,4-triazolo[1,5-a]pyrimidines for treatment of seizures and neurological disorders.

INVENTOR(S): Heal, David John; Fernandez, Fernandez Maria Isab;
 Sargent, Bruce Jeremy

PATENT ASSIGNEE(S): Boots Co. PLC, UK

SOURCE: PCT Int. Appl., 80 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

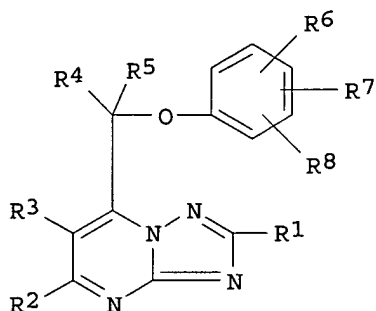
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9510521	A1	19950420	WO 1994-EP3364	19941012
W: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LU, LV, MD, MG, MN, MW, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SI, SK, TJ, TT, UA, US, UZ				
RW: KE, MW, SD, SZ, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
IN 179169	A	19970906	IN 1994-MA982	19941011
CA 2173857	AA	19950420	CA 1994-2173857	19941012
AU 9478554	A1	19950504	AU 1994-78554	19941012
AU 679573	B2	19970703		
ZA 9407949	A	19960123	ZA 1994-7949	19941012
EP 723546	A1	19960731	EP 1994-929537	19941012

EP 723546	B1	20000119		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
CN 1135754	A	19961113	CN 1994-194265	19941012
CN 1040537	B	19981104		
HU 74580	A2	19970128	HU 1996-959	19941012
JP 09503771	T2	19970415	JP 1994-511287	19941012
BR 9407812	A	19970506	BR 1994-7812	19941012
IL 111259	A1	19980208	IL 1994-111259	19941012
RU 2136684	C1	19990910	RU 1996-108927	19941012
PL 177920	B1	20000131	PL 1994-313970	19941012
ES 2142413	T3	20000416	ES 1994-929537	19941012
RO 117020	B1	20010928	RO 1996-795	19941012
SK 282329	B6	20020107	SK 1996-437	19941012
NO 9601435	A	19960610	NO 1996-1435	19960411
FI 9601630	A	19960412	FI 1996-1630	19960412
US 5753665	A	19980519	US 1996-628662	19960625
IN 182801	A	19990724	IN 1996-MA1544	19960904
GR 3032480	T3	20000531	GR 2000-400175	20000126

PRIORITY APPLN. INFO.: GB 1993-21162 A 19931013
IN 1994-MA982 A1 19941011
WO 1994-EP3364 W 19941012

OTHER SOURCE(S): MARPAT 123:313997

GI



I

AB Title compds. [I; R1 = H, (substituted) alkyl, alkoxy, alkanoyl; R2, R3 = H, (substituted) alkyl, alkoxy, alkanoyl, alkylthio, alkylsulfinyl, alkylsulfonyl; R4, R5 = H, (substituted) alkyl; R4R5C = C3-6 (substituted) cycloalkylidene; R6, R7, R8 = H, halo, OH, SH, cyano, (substituted) alkyl, alkanoyl, alkoxy, alkoxycarbonyl, CO₂H, alkanoyloxy, alkylthio, alkylsulfinyl, alkylsulfonyl, alkylsulfonylamino, sulfamoyl, carbamoyl, alkylcarbamoyl, alkanoylamino] were prepared. Thus, 4-fluorophenol was stirred 30 min. with NaH in 1,2-dimethoxyethane; 7-(1-bromoethyl)-1,2,4-triazolo[1,5-a]pyrimidine (preparation given) in 1,2-dimethoxyethane was added and the mixture was stirred 24 h to give 7-[1-(4-fluorophenoxy)ethyl]-1,2,4-triazolo[1,5-a]pyrimidine. II antagonized (+)-bicuculline-induced myoclonic seizures in mice with ED₅₀ = 13.9 mg/kg orally. The activity of I may arise from the ability to potentiate transmission of GABA and/or the ability to activate potassium channels in **neurons**.

IC ICM C07D487-04

ICS A61K031-505

ICI C07D487-04, C07D249-00, C07D239-00

CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))

Section cross-reference(s): 1

IT 165383-11-9P 165383-12-0P 165383-13-1P

165383-14-2P 165383-15-3P 165383-16-4P
 165383-17-5P 165383-18-6P 165383-19-7P
 165383-20-0P 165383-21-1P 165383-22-2P
 165383-23-3P 165383-24-4P 165383-25-5P
 165383-26-6P 165383-27-7P 165383-28-8P
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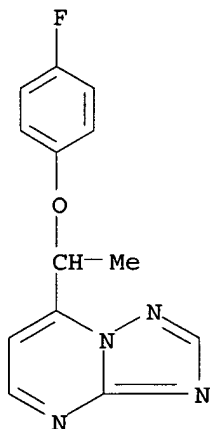
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (preparation of 7-phenoxyalkyl-1,2,4-triazolo[1,5-a]pyrimidines for treatment of seizures and neurol. disorders)

IT 165383-11-9P 165383-12-0P 165383-13-1P
 165383-14-2P 165383-15-3P 165383-16-4P
 165383-17-5P 165383-18-6P 165383-19-7P
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 165383-29-9P 165383-30-2P 165383-49-3P
 165383-50-6P 165383-51-7P 165383-52-8P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (preparation of 7-phenoxyalkyl-1,2,4-triazolo[1,5-a]pyrimidines for treatment of seizures and neurol. disorders)

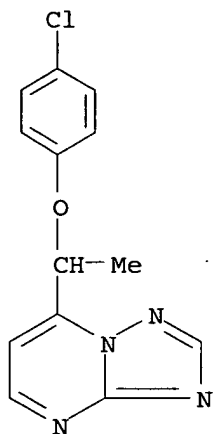
RN 165383-11-9 HCAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidine, 7-[1-(4-fluorophenoxy)ethyl]- (9CI) (CA INDEX NAME)



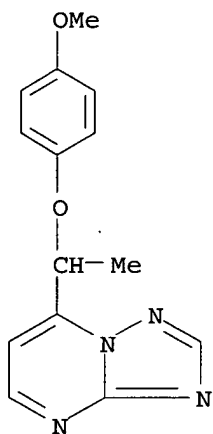
RN 165383-12-0 HCAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidine, 7-[1-(4-chlorophenoxy)ethyl]- (9CI) (CA INDEX NAME)



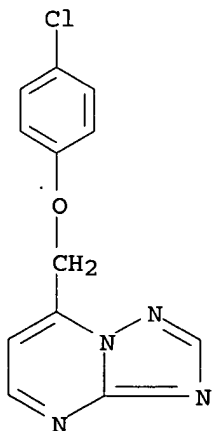
RN 165383-13-1 HCAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidine, 7-[1-(4-methoxyphenoxy)ethyl] - (9CI)
(CA INDEX NAME)

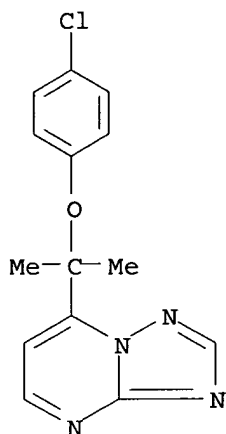


RN 165383-14-2 HCAPLUS

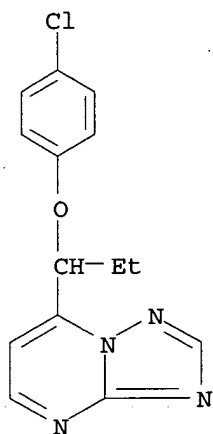
CN [1,2,4]Triazolo[1,5-a]pyrimidine, 7-[(4-chlorophenoxy)methyl] - (9CI) (CA
INDEX NAME)



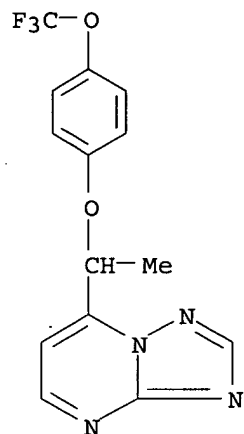
RN 165383-15-3 HCAPLUS
 CN [1,2,4]Triazolo[1,5-a]pyrimidine, 7-[1-(4-chlorophenoxy)-1-methylethyl]-
 (9CI) (CA INDEX NAME)



RN 165383-16-4 HCAPLUS
 CN [1,2,4]Triazolo[1,5-a]pyrimidine, 7-[1-(4-chlorophenoxy)propyl]- (9CI)
 (CA INDEX NAME)

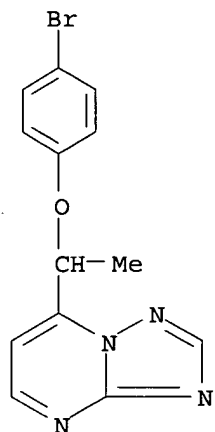


RN 165383-17-5 HCAPLUS
 CN [1,2,4]Triazolo[1,5-a]pyrimidine, 7-[1-[4-(trifluoromethoxy)phenoxy]ethyl]-
 (9CI) (CA INDEX NAME)



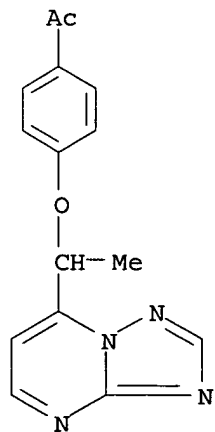
RN 165383-18-6 HCAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidine, 7-[1-(4-bromophenoxy)ethyl]- (9CI) (CA INDEX NAME)



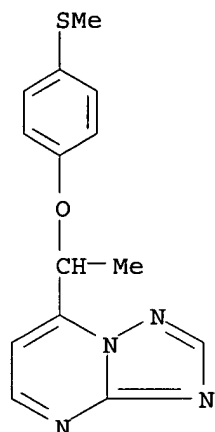
RN 165383-19-7 HCAPLUS

CN Ethanone, 1-[4-(1-[1,2,4]triazolo[1,5-a]pyrimidin-7-ylethoxy)phenyl]- (9CI) (CA INDEX NAME)



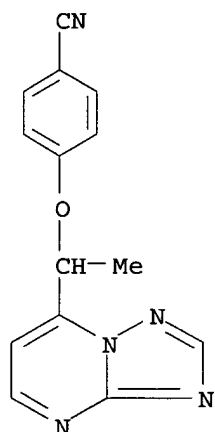
RN 165383-20-0 HCAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidine, 7-[1-[4-(methylthio)phenoxy]ethyl]-(9CI) (CA INDEX NAME)



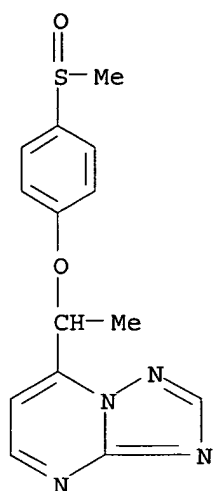
RN 165383-21-1 HCAPLUS

CN Benzonitrile, 4-(1-[1,2,4]triazolo[1,5-a]pyrimidin-7-ylethoxy)-(9CI) (CA INDEX NAME)



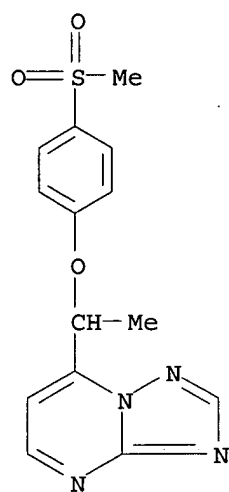
RN 165383-22-2 HCAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidine, 7-[1-[4-(methylsulfinyl)phenoxy]ethyl]-(9CI) (CA INDEX NAME)



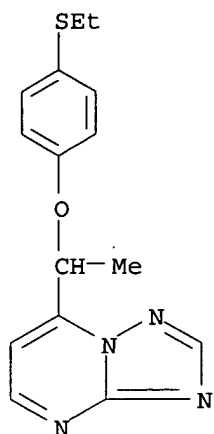
RN 165383-23-3 HCAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidine, 7-[1-[4-(methylsulfonyl)phenoxy]ethyl]-
(9CI) (CA INDEX NAME)



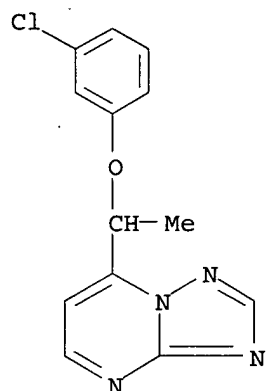
RN 165383-24-4 HCAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidine, 7-[1-[4-(ethylthio)phenoxy]ethyl]- (9CI)
(CA INDEX NAME)



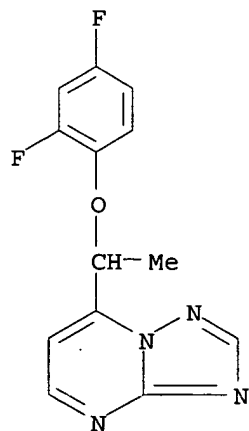
RN 165383-25-5 HCAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidine, 7-[1-(3-chlorophenoxy)ethyl] - (9CI) (CA INDEX NAME)



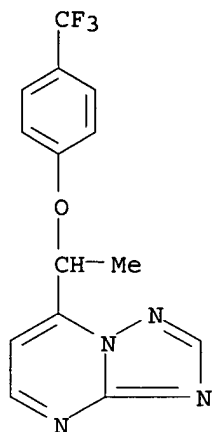
RN 165383-26-6 HCAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidine, 7-[1-(2,4-difluorophenoxy)ethyl] - (9CI) (CA INDEX NAME)



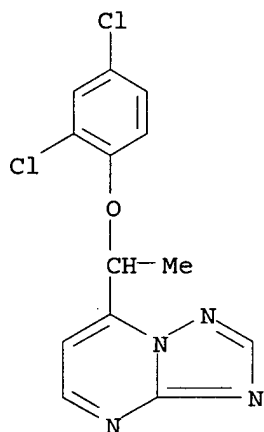
RN 165383-27-7 HCAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidine, 7-[1-[4-(trifluoromethyl)phenoxy]ethyl]- (9CI) (CA INDEX NAME)



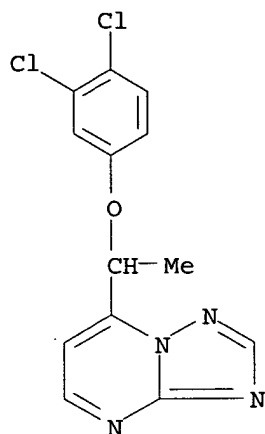
RN 165383-28-8 HCAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidine, 7-[1-(2,4-dichlorophenoxy)ethyl]- (9CI) (CA INDEX NAME)



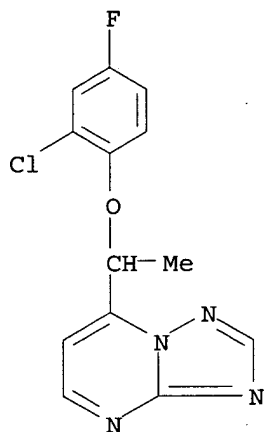
RN 165383-29-9 HCAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidine, 7-[1-(3,4-dichlorophenoxy)ethyl]- (9CI) (CA INDEX NAME)



RN 165383-30-2 HCAPLUS

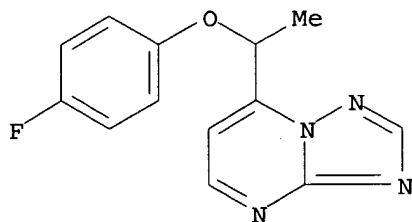
CN [1,2,4]Triazolo[1,5-a]pyrimidine, 7-[1-(2-chloro-4-fluorophenoxy)ethyl]-
(9CI) (CA INDEX NAME)



RN 165383-49-3 HCAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidine, 7-[1-(4-fluorophenoxy)ethyl]-, (+)-
(9CI) (CA INDEX NAME)

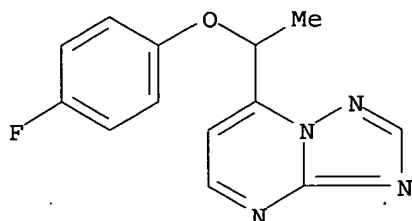
Rotation (+).



RN 165383-50-6 HCAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidine, 7-[1-(4-fluorophenoxy)ethyl]-, (-)-
(9CI) (CA INDEX NAME)

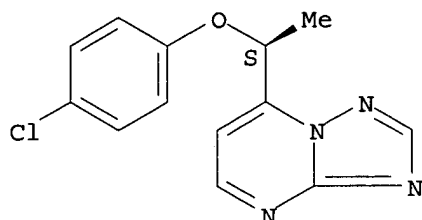
Rotation (-).



RN 165383-51-7 HCAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidine, 7-[(1S)-1-(4-chlorophenoxy)ethyl]- (9CI)
(CA INDEX NAME)

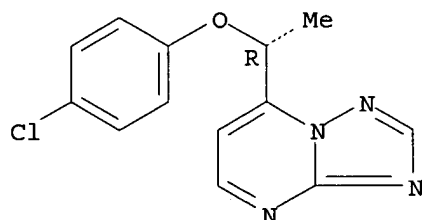
Absolute stereochemistry. Rotation (+).



RN 165383-52-8 HCAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidine, 7-[(1R)-1-(4-chlorophenoxy)ethyl]- (9CI)
(CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



L24 ANSWER 10 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1990:379 HCAPLUS

DOCUMENT NUMBER: 112:379

TITLE: Effect of trapidil (Rocornal) and its derivatives on the calcium current in cultured **neurones** and the effect of the trapidil derivative AR 12456 on contraction parameters of different cardiovascular preparations

AUTHOR(S): Bodewei, Rolf; Flederwisch, I.; Hering, S.; Schubert, B.; Warbanov, W.

CORPORATE SOURCE: Bereich. Zell. Mol. Kardiol., Wiss. DDR, Berlin, DDR-1115, Ger. Dem. Rep.

SOURCE: Wissenschaftliche Zeitschrift der Ernst-Moritz-Arndt-Universitaet Greifswald, Medizinische Reihe (1988),

37(2-3), 58-66

CODEN: WZERDH; ISSN: 0138-1067

DOCUMENT TYPE: Journal

LANGUAGE: German

AB The effects of trapidil and AR 12456 on Ca influx in cultured neuroblastoma-glioma hybrid cells and on contractility of rabbit heart and artery preps. and of neonatal rat heart cells were studied by electrophysiol methods. At relatively high concns. both agents had Ca-antagonist and neg. inotropic effects. There may be tissue-specific differences in Ca channel responses to trapidil and related compds.

CC 1-8 (Pharmacology)

ST trapidil AR 12456 calcium channel **neuron**; artery heart contraction trapidil AR 12456

IT 15421-84-8, Trapidil 100557-06-0, AR-12456

RL: BIOL (Biological study)

(heart and artery contractility and **neuronal** calcium influx response to)

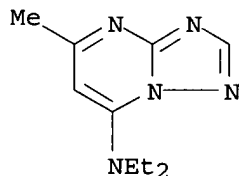
IT 15421-84-8, Trapidil

RL: BIOL (Biological study)

(heart and artery contractility and **neuronal** calcium influx response to)

RN 15421-84-8 HCAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidin-7-amine, N,N-diethyl-5-methyl- (9CI) (CA INDEX NAME)



L24 ANSWER 11 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1989:107854. HCAPLUS

DOCUMENT NUMBER: 110:107854

TITLE: Effects of trapidil and trapidil derivatives on arachidonic acid and prostaglandin endoperoxide analog U 46619-induced blood pressure changes in rats

AUTHOR(S): Heinroth-Hoffmann, I; Hauser, A.; Taube, C.; Mest, H. J.

CORPORATE SOURCE: Dep. Pharmacol. Toxicol., Martin Luther Univ., Halle, 4020, Ger. Dem. Rep.

SOURCE: Biomedica Biochimica Acta (1989), 47(10-11), S145-S148
CODEN: BBIADT; ISSN: 0232-766X

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The influence of trapidil (T) and two 5,7-disubstituted 1,2,4-triazolo[1,5-a]pyrimidine derivs. (TD, AR 12456 and AR 12463) on blood pressure changes induced by arachidonic acid (AA) and the prostaglandin endoperoxide analog U 46619 was studied in normotensive rats in comparison with the effects of the cyclooxygenase inhibitor acetylsalicylic acid (ASA) and the TXA2 antagonist BM 13177. ASA and AR 12456 completely eliminated the second blood pressure depression after injection of AA and simultaneously diminished TXA2, TXB2 and 6-keto-PGF1 α formation in murine blood, whereas BM 13177 prevented

the return of the blood pressure to the preinjection level after the initial brief fall in arterial pressure. BM 13177 and AR 12463 reduced the rise in U 46619-provoked blood pressure by 75 and 58%, resp. Trapidil had no effect on blood pressure changes stimulated by AA and U 46619.

CC 1-8 (Pharmacology)

IT 15421-84-8, Trapidil 100557-04-8, AR 12463 100557-06-0, AR 12456

RL: BIOL (Biological study)

(blood pressure response to arachidonic acid and U-46619 modulation by)

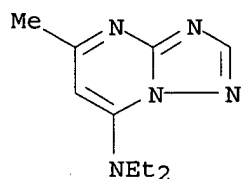
IT 15421-84-8, Trapidil

RL: BIOL (Biological study)

(blood pressure response to arachidonic acid and U-46619 modulation by)

RN 15421-84-8 HCAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidin-7-amine, N,N-diethyl-5-methyl- (9CI) (CA INDEX NAME)



L24 ANSWER 12 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1976:413792 HCAPLUS

DOCUMENT NUMBER: 85:13792

TITLE: Pharmacology of trapymine. 2. Analysis of the mode of action

AUTHOR(S): Ohnishi, Haruo; Tsukuda, Shigeru; Yamaguchi, Kazuo; Ogawa, Nobuhisa; Uchiyama, Toshimitsu; Ito, Ryuta

CORPORATE SOURCE: Res. Lab. Pharmacol., Mochida Pharm. Co., Ltd., Tokyo, Japan

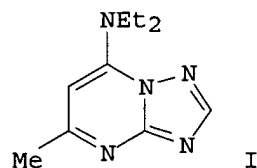
SOURCE: Nippon Yakurigaku Zasshi (1975), 71(7), 727-38

CODEN: NYKZAU; ISSN: 0015-5691

DOCUMENT TYPE: Journal

LANGUAGE: Japanese

GI



AB Trapymin (I) [15421-84-8] (10-5-10-4M) relaxed the isolated renal, pulmonary, femoral, and mesenteric arteries in rabbits, and coronary arteries in pigs. These relaxations were not antagonized by propranolol.

I was effective on vasopressin-induced angina in rats and electrocoagulation-induced myocardial infarction in rabbits, and suppressed adrenaline-induced arrhythmia but not CaCl_2 -induced arrhythmia in rats. I reduced catechol amine content in brain, adrenals, and heart, but had no effect on monoamine oxidase in brain and liver of rats. I showed ganglion-blocking and **neuron**-blocking effects on cervical ganglions in cats. Na^+ -, K^+ -dependent ATPase of bovine heart and P/O ratio of mitochondria of rat heart were not affected by I. The action of I is papaverine [58-74-2]-like and mediated by β -receptors.

CC 1-5 (Pharmacodynamics)

IT 15421-84-8

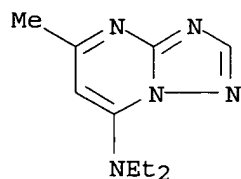
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(pharmacol. of)

IT 15421-84-8

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(pharmacol. of)

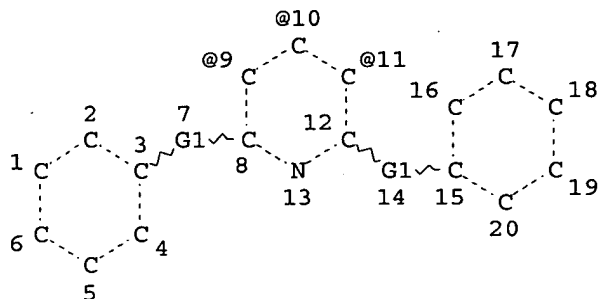
RN 15421-84-8 HCAPLUS

CN [1,2,4]Triazolo[1,5-a]pyrimidin-7-amine, N,N-diethyl-5-methyl- (9CI) (CA INDEX NAME)



=> d que
L25

STR



S @21

S ~ O
@22 23

G2 @24

Ak @25 O @26 S @27 N @28

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VAR G2=25/26/27/28/NO2/CN
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GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 28

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STEREO ATTRIBUTES: NONE
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L28 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2004:41501 HCAPLUS
DOCUMENT NUMBER: 140:87744
TITLE: Affinity small molecules for the EPO receptor
INVENTOR(S): Olsson, Lennart; Naranda, Tatjana
PATENT ASSIGNEE(S): Receptron, Inc., USA
SOURCE: PCT Int. Appl., 85 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004005323	A2	20040115	WO 2003-US21394	20030703
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				

PRIORITY APPLN. INFO.:
 US 2002-393360P P 20020703
 US 2002-393361P P 20020703
 US 2002-394110P P 20020703

OTHER SOURCE(S): MARPAT 140:87744

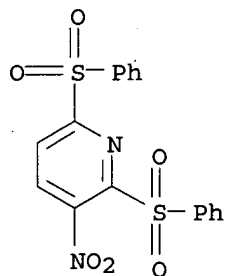
AB Comps. are provided that complex with the modulating domain of erythropoietin receptor (EPO-R) for use with EPO-R to determine the presence of EPO-R, the ability of other mols. to bind to the modulating domain in competitive assays and to induce a signal by EPO-R into a cell when bound by the subject comps. in a physiol. environment. The comps. are characterized by having a six-membered heterocyclic ring comprising at least one nitrogen atom and include substituted triazolopyrimidine, pyridazinone, pyridine and piperidine.

IT 259683-29-9

RL: BSU (Biological study, unclassified); BUU (Biological use, unclassified); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
 (affinity small mols. for erythropoietin (EPO) receptor and EPO receptor modulating sequence in relation to modulating the response to the stimulus of hematopoietic or neuronal cells and treatment of anemia)

RN 259683-29-9 HCAPLUS

CN Pyridine, 3-nitro-2,6-bis(phenylsulfonyl)- (9CI) (CA INDEX NAME)



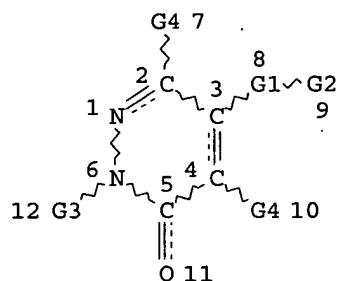
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Ward PCT/US03/21394

=> d que l32

L29

STR



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@14 15

N @16

Cb @17

Hy @18

Hy @19

Ak @20

O @21

NH^S
@22 23

Ak @24

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VAR G2=17/18/19

VAR G3=H/20

VAR G4=H/21/22/NO2/CN/24

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CONNECT IS E1 RC AT 15

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CONNECT IS E1 RC AT 24

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

ECOUNT IS E6 C AT 17

ECOUNT IS E4 C E2 N AT 18

ECOUNT IS E5 C E1 N AT 19

ECOUNT IS X3 C AT 20

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 24

STEREO ATTRIBUTES: NONE

L31 29 SEA FILE=REGISTRY SSS FUL L29

L32 14 SEA FILE=HCAPLUS ABB=ON PLU=ON L31

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L32 ANSWER 1 OF 14 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2002:623925 HCAPLUS

DOCUMENT NUMBER: 138:106662

TITLE: Synthesis of [1,4]benzodioxino[2,3-c and
2,3-d]pyridazinones

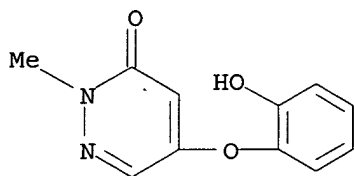
AUTHOR(S): Chung, Hyun-A.; Kim, Jeum-Jong; Cho, Su-Dong; Lee,
Sang-Gyeong; Yoon, Yong-Jin; Kim, Sung-Kyu

CORPORATE SOURCE: Department of Chemistry and Research Institute of

Searched by Paul Schulwitz

Natural Sciences College of Natural Sciences,
Gyeongsang National University, Jinju, 660-701, S.
Korea

SOURCE: Journal of Heterocyclic Chemistry (2002), 39(4),
685-689
CODEN: JHTCAD; ISSN: 0022-152X
PUBLISHER: HeteroCorporation
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:106662
AB Reaction of chloropyridazin-3-ones with catechol in the presence of
potassium carbonate gave the corresponding [1,4]benzodioxino[2,3-c and/or
2,3-d]pyridazinones.
IT **485808-28-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of benzodioxinopyridazinones via reaction of catechol with
chloropyridazinones in presence of potassium carbonate catalyst)
RN 485808-28-4 HCAPLUS
CN 3(2H)-Pyridazinone, 5-(2-hydroxyphenoxy)-2-methyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 2 OF 14 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1998:645926 HCAPLUS

DOCUMENT NUMBER: 129:302606

TITLE: Dehalogenation of 1-methyl-5-halo-4-substituted-
pyridazin-6-ones

AUTHOR(S): Kweon, Deok-Heon; Kang, Young-Jin; Chung, Hyun-A.;
Yoon, Yong-Jin

CORPORATE SOURCE: Department of Chemistry & Research Institute of
Natural Sciences, Gyeongsang National University,
Jinju, 660-701, S. Korea

SOURCE: Journal of Heterocyclic Chemistry (1998), 35(4),
819-826

CODEN: JHTCAD; ISSN: 0022-152X

PUBLISHER: HeteroCorporation

DOCUMENT TYPE: Journal

LANGUAGE: English

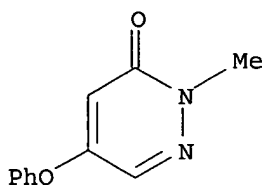
AB In order to confirm the regiochem. for the functionalization of
1-(1,1-dibromo-2-oxopropyl)-4,5-dihalopyridazin-6-ones, the dehalogenation
of 1-methyl-5-halo-4-substituted-pyridazin-6-ones using Pd/C and hydrogen
was carried out. The results of the title reaction are reported.

IT **214556-22-6P 214556-23-7P**

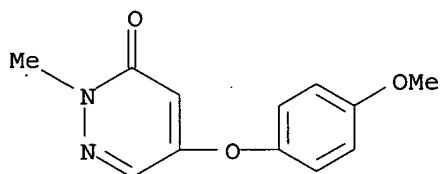
RL: SPN (Synthetic preparation); PREP (Preparation)
(dehalogenation of halopyridazinones)

RN 214556-22-6 HCAPLUS

CN 3(2H)-Pyridazinone, 2-methyl-5-phenoxy- (9CI) (CA INDEX NAME)



RN 214556-23-7 HCAPLUS
CN 3 (2H)-Pyridazinone, 5-(4-methoxyphenoxy)-2-methyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 3 OF 14 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1997:521682 HCAPLUS

DOCUMENT NUMBER: 127:214594

TITLE: Pharmacophore requirements in new series of pyridazinyl alkanolic acids, N-[(pyridazin-2-yl) alkyl] succinyl and glutaryl amides, inhibitors of thromboxane A2 biosynthesis

AUTHOR(S): Moreau, S.; Coudert, P.; Lasserre, B.; Vallee-Goyet, D.; Gardette, D.; Navarro-Delmasure, C.; Chanh, A. Pham Huu; Dossou-Gbete, V.; Couquelet, J.

CORPORATE SOURCE: Groupe de Recherches en Pharmacochimie Laboratoire de Chimie Therapeutique Faculte de Pharmacie 28, Clermont-Ferrand, F-63001, Fr.

SOURCE: Prostaglandins, Leukotrienes and Essential Fatty Acids (1997), 56(6), 431-436

CODEN: PLEAEU; ISSN: 0952-3278

PUBLISHER: Churchill Livingstone

DOCUMENT TYPE: Journal

LANGUAGE: English

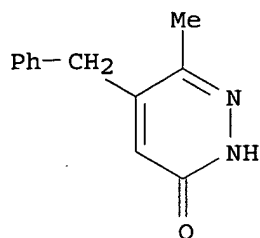
AB New series of 5-benzyl-6-methyl-4-oxo pyridazin-2-yl alkanolic acids, N-[(pyridazin-2-yl)alkyl] succinyl and glutaryl amides have been synthesized and evaluated in vitro as TXA2 biosynthesis inhibitors. The expts. were carried out using arachidonic acid (32.8 μ M) as a substrate and horse platelet microsomes as sources of TXA2 synthase. The presence of TXB2, a stable metabolite of TXA2, was determined by RIA. The potency of active compds. ($1.10^{-4} < IC_{50} < 1.10^{-6}$ M) greatly depends on the length of the chain at the N-2 position on the pyridazine ring. Furthermore, enzyme inhibition in vitro is increased with the presence of a halogen atom on the aromatic moiety of the benzyl group at C-5. The compound having a pentanoic side chain and a 4-fluoro benzyl moiety was the most active derivative with an IC_{50} value of 6.69×10^{-6} M. Mol. modeling studies were done on all the synthesized pyridazinones and on prostaglandin H2 (PGH2) suggesting spatial features and vols. of TXA2 synthase pharmacophore mode in these series of derivs.

IT 173429-17-9

RL: RCT (Reactant); RACT (Reactant or reagent)
 (reactant; pharmacophore requirements in a new series of pyridazinyl
 alkanolic acids as inhibitors of thromboxane A2 biosynthesis)

RN 173429-17-9 HCAPLUS

CN 3(2H)-Pyridazinone, 6-methyl-5-(phenylmethyl)- (9CI) (CA INDEX NAME)



L32 ANSWER 4 OF 14 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1996:623003 HCAPLUS

DOCUMENT NUMBER: 125:238690

TITLE: Ligands for the SH2 domain of the src protein for
 treatment of bone resorption diseases

INVENTOR(S): Dunnington, Damien John

PATENT ASSIGNEE(S): Smithkline Beecham Corporation, USA

SOURCE: Eur. Pat. Appl., 46 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 4

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 727211	A1	19960821	EP 1996-200270	19960207
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
AU 9644404	A1	19960822	AU 1996-44404	19960207
ZA 9601000	A	19960807	ZA 1996-1000	19960208
CA 2169136	AA	19960811	CA 1996-2169136	19960208
ZA 9601001	A	19960813	ZA 1996-1001	19960208
CN 1135333	A	19961113	CN 1996-104364	19960208
CN 1137378	A	19961211	CN 1996-105740	19960208
JP 09087200	A2	19970331	JP 1996-59921	19960208
CA 2212645	AA	19960815	CA 1996-2212645	19960209
WO 9624343	A1	19960815	WO 1996-US1964	19960209
W: AM, AU, BB, BG, BR, BY, CA, CN, CZ, EE, FI, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LV, MD, MG, MN, MX, NO, NZ, PL, PT, RO, RU, SD, SG, SI, SK, TJ, TM, TR, TT, UA, US, UZ, VN				
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9649237	A1	19960827	AU 1996-49237	19960209
EP 809490	A1	19971203	EP 1996-905494	19960209
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI				
BR 9607614	A	19980609	BR 1996-7614	19960209
JP 10513474	T2	19981222	JP 1996-524486	19960209
WO 9624847	A1	19960815	WO 1996-US2490	19960212

W: JP, US

RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE

EP 811159 A1 19971210 EP 1996-906615 19960212

R: BE, CH, DE, DK, FR, GB, IT, LI, NL

JP 10513564 T2 19981222 JP 1996-524493 19960212

ZA 9601318 A 19970127 ZA 1996-1318 19960220

ZA 9605499 A 19980330 ZA 1996-5499 19960628

ZA 9605500 A 19980330 ZA 1996-5500 19960628

FI 9703259 A 19971008 FI 1997-3259 19970807

NO 9703659 A 19971008 NO 1997-3659 19970808

PRIORITY APPLN. INFO.:

US 1995-386381 A 19950210

US 1995-400220 A 19950307

US 1995-497357 A 19950630

US 1995-541080 A 19951011

US 1995-580868 19951229

WO 1996-US1964 W 19960209

WO 1996-US2490 W 19960212

AB A method of treating a bone resorption disease by administering a compound that binds to the SH2 domain of the human src, e.g. I, protein with a binding affinity greater than 50-fold higher than for the SH2 domains of the human lck, fyn, hcp, Grb2, SH-PTP2, and p85 is described. The preparation of a number of compds. is described. An assay system for binding of these ligands to SH2 domains using SH2 domains manufactured as fusion proteins in Escherichia coli is described. I inhibited inhibited 45Ca in a mouse embryonic ulna model with an IC50 of 19 μ M.

IT 182198-18-1P

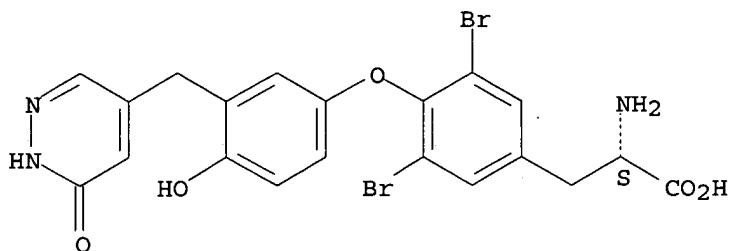
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of, as ligand for SH2 domain of src protein; ligands for SH2 domain of src protein for treatment of bone resorption diseases)

RN 182198-18-1 HCAPLUS

CN L-Tyrosine, 3,5-dibromo-O-[3-[(1,6-dihydro-6-oxo-4-pyridazinyl)methyl]-4-hydroxyphenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L32 ANSWER 5 OF 14 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1995:871851 HCAPLUS

DOCUMENT NUMBER: 124:86262

TITLE: Heterocyclic tautomerism. IX. Structural revision of a series of pharmacologically active pyridazines

AUTHOR(S): Guard, James A. M.; Steel, Peter J.

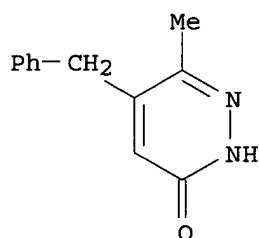
CORPORATE SOURCE: Chemistry Dep., Univ. Canterbury, Christchurch, N. Z.

SOURCE: Australian Journal of Chemistry (1995), 48(9), 1601-7

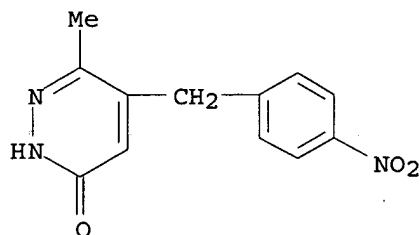
CODEN: AJCHAS; ISSN: 0004-9425

PUBLISHER: Commonwealth Scientific and Industrial Research Organization

DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB On the basis of ^1H NMR n.O.e. measurements and an x-ray crystal structure determination, it is shown that a large series of pharmacol. active pyridazine derivs. should be represented as aromatic pyridazine tautomers [e.g. (1b)-(3b)], rather than the previously reported arylidene-4,5-dihydropyridazines [e.g. (1a)-(3a)]. Crystals of (7b) are monoclinic, $P2_1/c$, a 13.312(3), b 7.269(1), c 11.753(2) Å, β 101.38(3)°, $Z = 4$; the structure was refined to a conventional $R[I > 2\sigma(I)]$ 0.037.
 IT 173429-17-9
 RL: PRP (Properties)
 (structural revision of pharmacol. active pyridazines as tautomers)
 RN 173429-17-9 HCAPLUS
 CN 3(2H)-Pyridazinone, 6-methyl-5-(phenylmethyl)- (9CI) (CA INDEX NAME)



IT 172606-32-5P
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (structural revision of pharmacol. active pyridazines as tautomers)
 RN 172606-32-5 HCAPLUS
 CN 3(2H)-Pyridazinone, 6-methyl-5-[(4-nitrophenyl)methyl]- (9CI) (CA INDEX NAME)



L32 ANSWER 6 OF 14 HCAPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 1995:840619 HCAPLUS
 DOCUMENT NUMBER: 123:271334
 TITLE: 5-(2-Chlorobenzyl)-6-methyl-3(2H)-pyridazinone
 AUTHOR(S): Moreau, Stephane; Metin, Jacques; Coudert, Pascal; Couquelet, Jacques
 CORPORATE SOURCE: Groupe Recherche Pharmacochimie, Lab. Chimie
 Therapeutique, Clermont-Ferrand, 63001, Fr.
 SOURCE: Acta Crystallographica, Section C: Crystal Structure
 Communications (1995), C51(9), 1834-6
 CODEN: ACSCEE; ISSN: 0108-2701

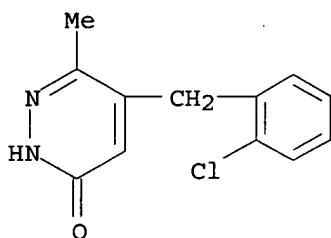
PUBLISHER: Munksgaard
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The title compound is monoclinic, space group P2₁, with a 7.270(1), b 7.076(4), c 11.227(1) Å, and β 100.57(1)°; Z = 2, d_c = 1.373, d_m = 1.2; R = 0.051, R_w = 0.054 for 1468 reflections. Atomic coordinates are given. The two planar rings (pyridazine and phenyl) are at an angle of .apprx.95°. Crystal cohesion is ensured by a dense network of van der Waals contacts.

IT 169136-07-6, 5-(2-Chlorobenzyl)-6-methyl-3(2H)-pyridazinone
RL: PRP (Properties)
(crystal structure of)

RN 169136-07-6 HCAPLUS

CN 3(2H)-Pyridazinone, 5-[(2-chlorophenyl)methyl]-6-methyl- (9CI) (CA INDEX NAME)



L32 ANSWER 7 OF 14 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1994:534057 HCAPLUS

DOCUMENT NUMBER: 121:134057

TITLE: Studies on pyridazinone derivatives. XVI.
Analgesic-antiinflammatory activities of
3(2H)-pyridazinone derivatives

AUTHOR(S): Takaya, Masahiro; Sato, Makoto

CORPORATE SOURCE: Hamari Chem. Co., Ltd., Osaka, 533, Japan

SOURCE: Yakugaku Zasshi (1994), 114(2), 94-110

CODEN: YKKZAJ; ISSN: 0031-6903

DOCUMENT TYPE: Journal

LANGUAGE: Japanese

AB In order to examine analgesic and antiinflammatory activities of the position isomers of 4-ethoxy-2-methyl-5-morpholino-3(2H)-pyridazinone (emorfazone), an analgesic-antiinflammatory drug, 5-ethoxy-2-methyl-4-morpholino-3(2H)-pyridazinone, 6-ethoxy-2-methyl-4-morpholino-3(2H)-pyridazinone and 6-ethoxy-2-methyl-5-morpholino-3(2H)-pyridazinone (I) were prepared. Since I showed the most strong activity among the compds. tested, various 6-alkoxy- or 6-allyloxy-2-alkyl- or 2-cyclohexyl- or 2-phenyl-5-substituted amino-3(2H)-pyridazinones were prepared and examined for their activities. As a result, I and 2-methyl-5-morpholino-6-n-propoxy- or 6-n-butoxy-3(2H)-pyridazinone and 6-ethoxy-2-ethyl-5-morpholino-3(2H)-pyridazinone were revealed to be more potent in analgesic and antipyretic activities than com. drugs (emorfazone, aminopyrine, mepirizole, tiaramide HCl, phenylbutazone, mefenamic acid). On the basis of the available data, the structure-activity relationship in a series of 6-alkoxy-2-alkyl-5-substituted amino-3(2H)-pyridazinones was also discussed.

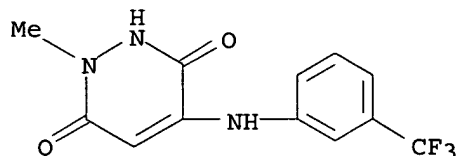
IT 88804-54-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)
(preparation and alkylation of)

RN 88804-54-0 HCAPLUS

CN 3,6-Pyridazinedione, 1,2-dihydro-1-methyl-4-[[3-(trifluoromethyl)phenyl]amino]- (9CI) (CA INDEX NAME)



L32 ANSWER 8 OF 14 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1989:38946 HCAPLUS

DOCUMENT NUMBER: 110:38946

TITLE: Studies on pyridazinone derivatives. XIII. Unusual displacement reaction of 5-(o-aminophenylthio)-4-chloro-2-methyl-3(2H)-pyridazinone with alkali

AUTHOR(S): Takaya, Masahiro

CORPORATE SOURCE: Hamari Chem. Co., Ltd., Osaka, 533, Japan

SOURCE: Yakugaku Zasshi (1988), 108(2), 136-41

CODEN: YKKZAJ; ISSN: 0031-6903

DOCUMENT TYPE: Journal

LANGUAGE: Japanese

OTHER SOURCE(S): CASREACT 110:38946

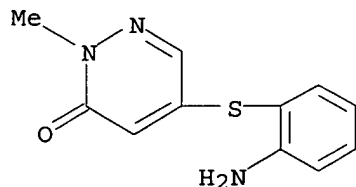
AB In order to explore the scope of an unusual displacement reaction to form 3-phenyl-10H-benzo[b]pyridazino[4,5-e][1,4]thiazine-4(3H)-one in the reaction of 5-(o-aminophenylthio)-4-chloro-2-phenyl-3(2H)-pyridazinone with NaOEt, the behavior of 2-Me (I) or 2-hydropyridazone derivs. (II) against NaOEt or NaOH were examined. Among them, I underwent an unusual displacement reaction to afford 3-methylthiazine derivative (III), 4-(o-aminophenylthio)-5-ethoxy-2-methyl-3(2H)-pyridazinone or 4-(o-aminophenylthio)-5-hydroxy-2-methyl-3(2H)-pyridazinone, but II did not.

IT 118327-46-1

RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclization-rearrangement of)

RN 118327-46-1 HCAPLUS

CN 3(2H)-Pyridazinone, 5-[(2-aminophenyl)thio]-2-methyl- (9CI) (CA INDEX NAME)



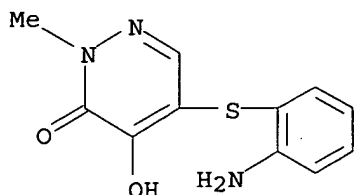
IT 51834-53-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)

(preparation and thermolysis of)

RN 51834-53-8 HCAPLUS

CN 3(2H)-Pyridazinone, 5-[(2-aminophenyl)thio]-4-hydroxy-2-methyl- (9CI) (CA INDEX NAME)

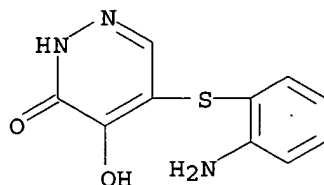


IT 118327-49-4

RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction with aqueous sodium hydroxide and thermolysis of)

RN 118327-49-4 HCAPLUS

CN 3(2H)-Pyridazinone, 5-[(2-aminophenyl)thio]-4-hydroxy- (9CI) (CA INDEX NAME)



L32 ANSWER 9 OF 14 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1988:528933 HCAPLUS

DOCUMENT NUMBER: 109:128933

TITLE: Synthesis of monochloromaleic hydrazide derivatives.
2. Substitution of methanethiol for chlorine

AUTHOR(S): Tonegawa, Masami; Nishimura, Yukihiro; Fukasawa, Chiyoko; Kitahara, Keiichi; Yamashita, Junzo; Sato, Hisao

CORPORATE SOURCE: Tokyo Med. Coll., Tokyo, Japan

SOURCE: Tokyo Ika Daigaku Kiyo (1988), 14, 1-11

CODEN: TIDKD9; ISSN: 0385-1303

DOCUMENT TYPE: Journal

LANGUAGE: Japanese

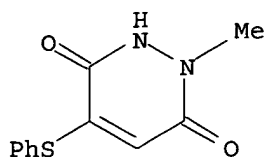
AB Substitution reactions of the title hydrazides I (R = Cl; R1 = Me, R2 = H, Me) and II (R = Cl; R1 = Me, R2 = H, Me; R1 = H, R2 = Me) with MeSNa gave the corresponding chlorine substitution products I and II (R = SMe), resp. In contrast, substitution of 4-chloro derivative I (R = Cl, R1 = H, R2 = Me) (III) with MeSNa or EtSNa gave a 1:1 mixture of 4- and 5-substituted derivs I and II (R = SMe, SEt, R1 = H, R2 = Me). Substitution of III with PhSNa gave only 4-substituted derivative I (R = SPh, R1 = H, R2 = Me).

IT 98045-61-5P

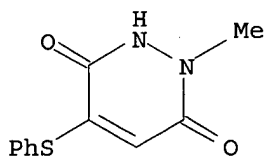
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 98045-61-5 HCAPLUS

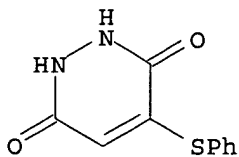
CN 3,6-Pyridazinedione, 1,2-dihydro-1-methyl-4-(phenylthio)- (9CI) (CA INDEX NAME)



L32 ANSWER 10 OF 14 HCAPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 1985:504905 HCAPLUS
 DOCUMENT NUMBER: 103:104905
 TITLE: Synthesis of monochloromaleic hydrazide derivatives.
 Synthesis of methylthio- and phenylthiomaleic
 hydrazides and their N-methyl and O-acyl derivatives
 AUTHOR(S): Satoh, Hisao; Tonegawa, Masami; Inoue, Reiko
 CORPORATE SOURCE: Dep. Chem., Tokyo Med. Coll., Tokyo, Japan
 SOURCE: Tokyo Ika Daigaku Kiyo (1985), 11, 1-12
 CODEN: TIDKD9; ISSN: 0385-1303
 DOCUMENT TYPE: Journal
 LANGUAGE: Japanese
 AB Reaction of chloromaleic hydrazide (I; R = 4-, 5-Cl; R1 = H) with MeSH or
 PhSH gave I (R = 4-, 5-MeS, -PhS; R1 = H), which were treated with Me2SO4
 to give N-Me derivs. (I; R = 4-, 5-MeS, -PhS; R1 = Me). Reaction of I (R
 = Cl, MeS, PhS; R1 = H) with PhCOCl/pyridine or Ac2O gave the
 corresponding benzoates or acetates (II; R2 = Ph, Me).
 IT **98045-61-5P**
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation and acylation of)
 RN 98045-61-5 HCAPLUS
 CN 3,6-Pyridazinedione, 1,2-dihydro-1-methyl-4-(phenylthio)- (9CI) (CA INDEX
 NAME)



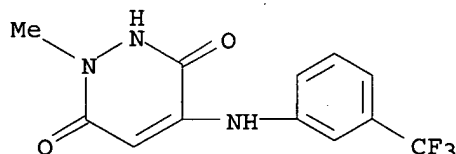
IT **98045-58-0P**
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation, methylation and acylation of)
 RN 98045-58-0 HCAPLUS
 CN 3,6-Pyridazinedione, 1,2-dihydro-4-(phenylthio)- (9CI) (CA INDEX NAME)



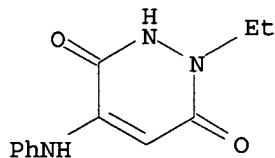
L32 ANSWER 11 OF 14 HCAPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 1984:85712 HCAPLUS
 DOCUMENT NUMBER: 100:85712
 TITLE: Pyridazines
 PATENT ASSIGNEE(S): Morishita Pharmaceutical Co., Ltd., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 5 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 58183675	A2	19831026	JP 1982-66742	19820420

PRIORITY APPLN. INFO.: JP 1982-66742 19820420
 OTHER SOURCE(S): CASREACT 100:85712
 AB The title compds. I [R = HO, alkoxy; R1 = alkyl; R2 = H, (halo) alkyl] were prepared by reaction of I (R = halo) with the appropriate Na or K hydroxides or alkoxides. Thus, refluxing a mixture of 2.4 g I (R = Cl, R1 = Me, R2 = H), 0.46 g Na, and 50 mL EtOH for 24 h gave 1.5 g I (R = EtO, R1 = Me, R2 = H).
 IT 88804-54-0P 88804-56-2P
 RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)
 RN 88804-54-0 HCAPLUS
 CN 3,6-Pyridazinedione, 1,2-dihydro-1-methyl-4-[[3-(trifluoromethyl)phenyl]amino]- (9CI) (CA INDEX NAME)



RN 88804-56-2 HCAPLUS
 CN 3,6-Pyridazinedione, 1-ethyl-1,2-dihydro-4-(phenylamino)- (9CI) (CA INDEX NAME)



L32 ANSWER 12 OF 14 HCAPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 1974:95822 HCAPLUS
 DOCUMENT NUMBER: 80:95822
 TITLE: Ring contraction of pyridazinones to pyrazols. VII
 AUTHOR(S): Maki, Yoshifumi; Suzuki, Mikio; Takaya, Masahiro
 CORPORATE SOURCE: Gifu Coll. Pharm., Gifu, Japan
 SOURCE: Chemical & Pharmaceutical Bulletin (1974), 22(1),

229-32

CODEN: CPBTAL; ISSN: 0009-2363

DOCUMENT TYPE:

Journal

LANGUAGE:

English

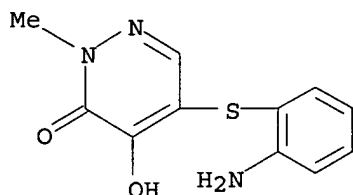
AB Previous results from the title ring contraction were extended to I. A suspension of I in 10% NaOH is heated several hr to yield II which on treatment with SOCl₂ in CHCl₃ is cyclized to III. An N₂-phenyl is necessary for this type of ring contraction.

IT 51834-53-8P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 51834-53-8 HCAPLUS

CN 3(2H)-Pyridazinone, 5-[(2-aminophenyl)thio]-4-hydroxy-2-methyl- (9CI) (CA
INDEX NAME)



L32 ANSWER 13 OF 14 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1962:456319 HCAPLUS

DOCUMENT NUMBER: 57:56319

ORIGINAL REFERENCE NO.: 57:11212b-i

TITLE: 1-Carbalkoxy-4-(aminoalkanol)piperazines

INVENTOR(S): Geschickter, Charles F.; Pierce, John S.; Chen, Ying
H.; Reid, Ebenezer E.

SOURCE: 5 pp.

DOCUMENT TYPE: Patent

LANGUAGE: Unavailable

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 301557		19620102	US	19590528

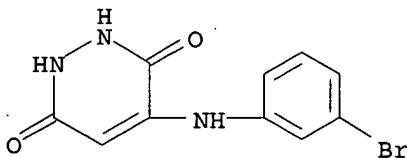
AB The title compds. (Ia) were prepared for use as inter-mediate in chemical syntheses. The Ia also had antitussive activity. A mixture of 0.05 mole 3-dibutylamino-1,2-epoxy-propane, 0.05 mole 1-carbopropoxypiperazine (I), and 50 ml. EtOH was allowed to stand 1 week, heated at 75° 8 hrs., and distilled to give 61% 1-carbopropoxy-4-(3-dibutylamino-2-hydroxy)piperazine, b0.12 162-4°. Allowing 0.029 mole I, 0.0:/9 mole epichlorohydrin, and 10 ml. EtOH to stand 14 hrs., adding NaOH, Me₂NH, and NaOH again (allowing the mixture to stand after each addition), and extracting with Et₂O gave 75% 1-carbopropoxy-4-(3-dimethylamino-2-hydroxypropyl)-piperazine, b0.4 144-6°. Also adding 1.8 g. Me chloroformate to 6.0 g. 1-(3-dibutylamino-2-hydroxy)-trans-2,5-dimethylpiperazine, 1 ml. Et₃N, and 60 ml. EtOH at 0°, adding NaOH, and extracting with Et₂O gave 30% 1-carbomethoxy-4-(3-dibutylamino-2-hydroxypropyl)-trans-2,5-dimethylpiperazine, b0.25 150-3°. By one or more of the above procedures the following Ia were prepared (n, B, R, and b.p./mm, given): 0, Et₂N, Me, 152-5°/0.4; 0, Et₂N, Et, 138-40°/0.2; 0, Et₂N, Pr, 155-7°/0.3; 0, Et₂N, Bu, 172-8°/0.4; 0, Bu₂N, Et, 175-9°/0.3; 0, Bu₂N, Pr,

162-4°/0.12; 0, Bu2N, Bu, 176-8°/0.2; 0, morpholino, Me,
 168-70°/0.45; 0, morpholino, Et, 205-11°/0.5; 0, morpholino,
 Bu, 200-5°/0.6; 0, pyrrolidino, Me, 164-7°/0.7; 0,
 pyrrolidino, Pr, 165-7°/ 0.25; 0, pyrrolidino, Bu,
 173-5°/0.7; 0, piperidino, Et, 173-7°/0.25; 0,
 2-methylpiperidino, Et, 184-6°/0.80; 0, 4-methylpiperidino, Me,
 168-71°/0.4; 0, 4-methylpiperidino, Et, 173-5°/0.35; 1,
 Me2N, Et, 192-3°/9.0; 1, Me2N, Pr, 148-50°/0.6; 1, Et2N, Et,
 162-5°/0.6; 1, Et2N, Bu, 180-5°/0.5; 1, Bu2N, Et,
 185-8°/0.3; 1, Bu2N, Pr, 200-2°/ 0.5; 1, Bu2N, Bu,
 181-2°/0.15; 1, morpholino, Me, 168-70°/0.25; 1, morpholino,
 Et, 210°/0.3; 1, morpholino, Bu, 197-8°/0.5; 1, pyrrolidino,
 Pr, 175-8°/0.45; 1, piperidino, Et, 174-83°/0.45; 1,
 piperidino, Pr, 187-9°/0.45; 1, 2-methylpiperidino, Bu,
 184-6°/0.3; 1, 3-methylpiperidino, Me, 175-8°/0.4; 1,
 4-methylpiperidino, Et, 178-80°/0.45; 2, Et2N, Bu,
 180-4°/0.5; 2, Et2N, Et, 161-6°/0-5; 2, Me2N, Bu,
 145-8°/0.5; 2, Et2N, Me, 155-7°/0.45; 2, Pr2N, Me,
 155-60°/0.25; 2, Pr2N, Et, 165-7°/0-35; 2, iso-Pr2N, Et,
 185-7°/0.45; 2, Bu2N, Me, 245-8°/8.0; 2, Bu2N, Et,
 173-5°/0.1; 2, Bu2N, Et, 188-90°/0-5; 2, Bu2N, Pr,
 168-70°/0.18; 2, Bu2N, Bu, 195-7°/0.1; 2, Bu2N, Bu,
 188-91°/0.35; 2, EtBuN, Bu, 176-8°/0.3; 2, morpholino, Me,
 175-7°/0.25; 2, morpholino, Et, 165-8°/ 0.25; 2,
 morpholino, Pr, 169-71°/0.15; 2, morpholino, Bu,
 210-12°/0.5; 2, pyrrolidino, Me 163-5°/0.35; 2, pyrrolidino,
 Et, 162-3°/0.45; 2, pyrrolidino, Pr, 180-2°/0.8; 2,
 piperidino, Et, 193°/0.2; 2, 2-methylpiperidino, Me,
 174-6°/0.30; 2, 2-methylpiperidino Et, 175-7°/0.45; 2,
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 182-5°/0.45; 2, 3-methylpiperidino, Me, 173-5°/0.45; 2,
 3-methylpiperidino, Et, 168-70°/0.25; 2, 4-methyl-piperidino, Bu,
 190-2°/0.3; 4, Me2N, Me, 145-7°/0.4; 4, Et2N, Me,
 163-5°/0.3; 4, Et2N, Et, 166-8°/0-35; 4, Bu2N, Me,
 179-5°/0.4; 4, morpholino, Me, 179-80°/0.5; 4, morpholino,
 Pr, 183-5°/0.4; 4, morpholino, Bu, 192-3°/0.45; 4
 pyrrolidino, Pr, 168-70°/0.35; 4, piperidino, Me,
 170-2°/0.45; 4, piperidino, Pr, 186-8°/0.5; 4,
 3-methylpiperidino, Bu, 182-5°/0.4; 4, 4-methylpiperidino, Et,
 180-2°/ 0.35; 4, 4-methylpiperidino, Bu, 190-4°/0.4.

IT 91211-30-2, 3,6-Pyridazinediol, 4-(m-bromoanilino)-
 (preparation of)

RN 91211-30-2 HCAPLUS

CN 3,6-Pyridazinediol, 4-(m-bromoanilino)- (7CI) (CA INDEX NAME)



L32 ANSWER 14 OF 14 HCAPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 1962:456318 HCAPLUS
 DOCUMENT NUMBER: 57:56318
 ORIGINAL REFERENCE NO.: 57:11211h-i,11212a-b

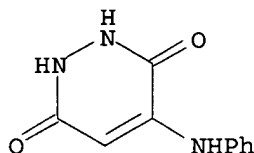
TITLE: N-(DihydroxypyridazinyI)aniline and derivatives thereof
 INVENTOR(S): Lowrie, Harman S.
 PATENT ASSIGNEE(S): G.D. Searle and Co.
 SOURCE: 2 pp.
 DOCUMENT TYPE: Patent
 LANGUAGE: Unavailable
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3037022		19620529	US	19600907

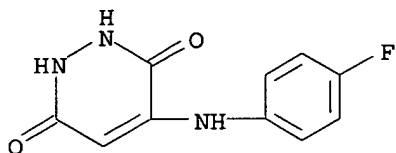
AB Comps. I are prepared by condensation of 4-chloro-3,6-dihydroxypyridazine (II) with the appropriately substituted aniline in the presence of Cu powder. Thus. a mixture of II 100, aniline 500, and Cu powder 1 part was rapidly heated to reflux. Refluxing was maintained for 25 min., the reaction mixture cooled to room temperature, and diluted with an equal volume of Et₂O.

The mixture was then extracted several times with dilute KOH, the exts. back-extracted with Et₂O, and then acidified with concentrated HCl. The solid, washed with H₂O, and recrystd. from MeOH, gave I (Z = H), m. 262-4° (decomposition). In the same manner were prepared the following I (Z given): 4-Me (m. 247-9° decomposition), 4-Et, 4-MeO [m. 225-30° (decomposition)], 4-EtO, 4-F [m. 272-4° (decomposition)], 4-Cl [m. 276-8° (decomposition)], 4-Br, 3-Me, 3-Et, 3-MeO, 3-EtO, 3-F, 3-Cl (m. 259-62°), and 3-Br. The I bare appetite-inhibiting and diuretic activity.

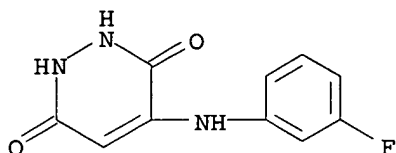
IT 90946-28-4, 3,6-Pyridazinediol, 4-anilino- (and derivs.)
 RN 90946-28-4 HCAPLUS
 CN 3,6-Pyridazinediol, 4-anilino- (7CI) (CA INDEX NAME)



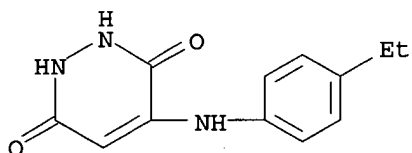
IT 782-69-4, 3,6-Pyridazinediol, 4-(p-fluoroanilino)-
 886-25-9, 3,6-Pyridazinediol, 4-(m-fluoroanilino)-
 88614-39-5, 3,6-Pyridazinediol, 4-(p-ethylanilino)-
 88617-78-1, 3,6-Pyridazinediol, 4-m-phenetidino-
 88617-79-2, 3,6-Pyridazinediol, 4-p-phenetidino-
 89126-21-6, 3,6-Pyridazinediol, 4-(m-ethylanilino)-
 90766-60-2, 3,6-Pyridazinediol, 4-(p-bromoanilino)-
 90799-86-3, 3,6-Pyridazinediol, 4-(p-chloroanilino)-
 91211-30-2, 3,6-Pyridazinediol, 4-(m-bromoanilino)-
 91587-72-3, 3,6-Pyridazinediol, 4-(m-chloroanilino)-
 92289-82-2, 3,6-Pyridazinediol, 4-p-toluidino- 92290-20-5
 , 3,6-Pyridazinediol, 4-p-anisidino- 93534-86-2,
 3,6-Pyridazinediol, 4-m-toluidino- 93534-91-9,
 3,6-Pyridazinediol, 4-m-anisidino- (preparation of)
 RN 782-69-4 HCAPLUS
 CN 3,6-Pyridazinediol, 4-(p-fluoroanilino)- (7CI, 8CI) (CA INDEX NAME)



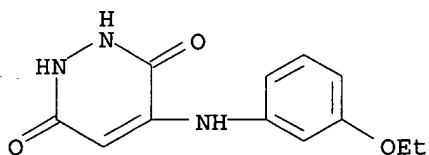
RN 886-25-9 HCAPLUS
CN 3,6-Pyridazinediol, 4-(m-fluoroanilino)- (7CI, 8CI) (CA INDEX NAME)



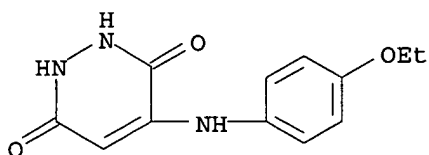
RN 88614-39-5 HCAPLUS
CN 3,6-Pyridazinediol, 4-(p-ethyl-anilino)- (7CI) (CA INDEX NAME)



RN 88617-78-1 HCAPLUS
CN 3,6-Pyridazinediol, 4-m-phenetidino- (7CI) (CA INDEX NAME)

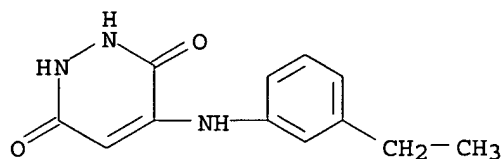


RN 88617-79-2 HCAPLUS
CN 3,6-Pyridazinediol, 4-p-phenetidino- (7CI) (CA INDEX NAME)



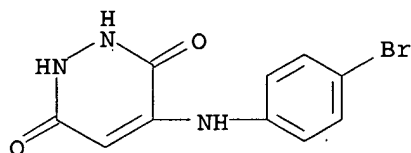
RN 89126-21-6 HCAPLUS

CN 3,6-Pyridazinediol, 4-(m-ethylanilino)- (7CI) (CA INDEX NAME)



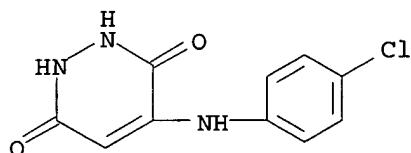
RN 90766-60-2 HCAPLUS

CN 3,6-Pyridazinediol, 4-(p-bromoanilino)- (7CI) (CA INDEX NAME)



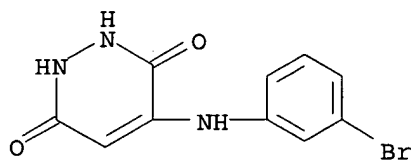
RN 90799-86-3 HCAPLUS

CN 3,6-Pyridazinediol, 4-(p-chloroanilino)- (7CI) (CA INDEX NAME)



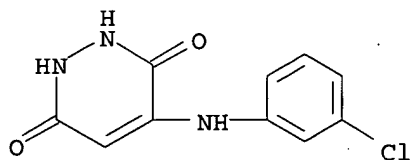
RN 91211-30-2 HCAPLUS

CN 3,6-Pyridazinediol, 4-(m-bromoanilino)- (7CI) (CA INDEX NAME)



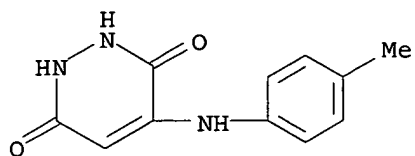
RN 91587-72-3 HCAPLUS

CN 3,6-Pyridazinediol, 4-(m-chloroanilino)- (7CI) (CA INDEX NAME)



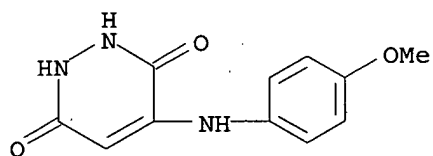
RN 92289-82-2 HCAPLUS

CN 3,6-Pyridazinediol, 4-p-toluidino- (7CI) (CA INDEX NAME)



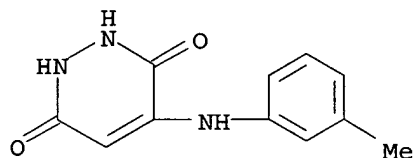
RN 92290-20-5 HCAPLUS

CN 3,6-Pyridazinediol, 4-p-anisidino- (7CI) (CA INDEX NAME)



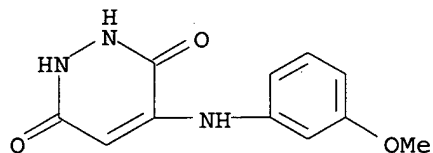
RN 93534-86-2 HCAPLUS

CN 3,6-Pyridazinediol, 4-m-toluidino- (7CI) (CA INDEX NAME)



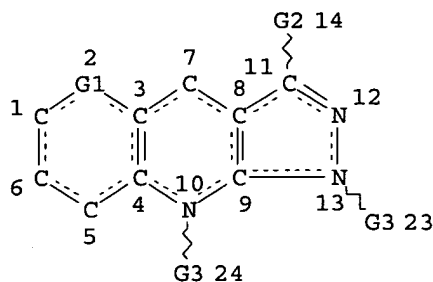
RN 93534-91-9 HCAPLUS

CN 3,6-Pyridazinediol, 4-m-anisidino- (7CI) (CA INDEX NAME)



L33

STR



C~Ak
@15 16

C=O
@17 18

C=S
@19 20

C @25

C=N
@21 22

VAR G1=CH2/15/17/19/21

VAR G2=H/25

VAR G3=H/C

NODE ATTRIBUTES:

NSPEC IS RC AT 25

CONNECT IS E3 RC AT 15

CONNECT IS E1 RC AT 16

CONNECT IS E1 RC AT 20

CONNECT IS E1 RC AT 22

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

ECOUNT IS X3 C AT 16

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 25

STEREO ATTRIBUTES: NONE

L35 52 SEA FILE=REGISTRY SSS FUL L33

L36 8 SEA FILE=HCAPLUS ABB=ON PLU=ON L35

=> d l36 ibib ab hitstr 1-8

L36 ANSWER 1 OF 8 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2004:41501 HCAPLUS

DOCUMENT NUMBER: 140:87744

TITLE: Affinity small molecules for the EPO receptor

INVENTOR(S): Olsson, Lennart; Naranda, Tatjana

PATENT ASSIGNEE(S): Receptron, Inc., USA

SOURCE: PCT Int. Appl., 85 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004005323	A2	20040115	WO 2003-US21394	20030703

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 2002-393360P P 20020703
US 2002-393361P P 20020703
US 2002-394110P P 20020703

OTHER SOURCE(S): MARPAT 140:87744

AB Compds. are provided that complex with the modulating domain of erythropoietin receptor (EPO-R) for use with EPO-R to determine the presence of EPO-R, the ability of other mols. to bind to the modulating domain in competitive assays and to induce a signal by EPO-R into a cell when bound by the subject compds. in a physiol. environment. The compds. are characterized by having a six-membered heterocyclic ring comprising at least one nitrogen atom and include substituted triazolopyrimidine, pyridazinone, pyridine and piperidine.

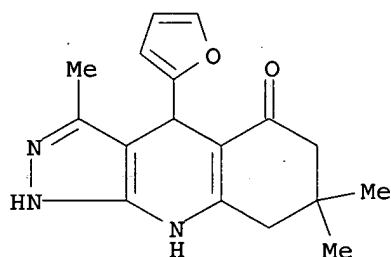
IT 645337-25-3

RL: BSU (Biological study, unclassified); BUU (Biological use, unclassified); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(affinity small mols. for erythropoietin (EPO) receptor and EPO receptor modulating sequence in relation to modulating the response to the stimulus of hematopoietic or neuronal cells and treatment of anemia)

RN 645337-25-3 HCAPLUS

CN 5H-Pyrazolo[3,4-b]quinolin-5-one, 4-(2-furanyl)-1,4,6,7,8,9-hexahydro-3,7,7-trimethyl- (9CI) (CA INDEX NAME)



L36 ANSWER 2 OF 8 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2001:826097 HCAPLUS

DOCUMENT NUMBER: 136:61813

TITLE: 4-(4-Chlorophenyl)-3,7,7-trimethyl-1-[2-(4-nitrobenzoyl)ethyl]-4,7,8,9-tetrahydro-1H-pyrazolo[3,4-b]quinolin-5(6H)-one-ethanol (1/1)

AUTHOR(S): Low, John Nicolson; Cobo, Justo; Nogueras, Manuel; Sanchez, Adolfo; Quiroga, Jairo; Mejia, Diana

CORPORATE SOURCE: Department of Chemistry, University of Aberdeen, Meston Walk, Old Aberdeen, AB24 3UE, UK

SOURCE: Acta Crystallographica, Section C: Crystal Structure Communications (2001), C57(11), 1356-1358

CODEN: ACSCEE; ISSN: 0108-2701

PUBLISHER: Munksgaard International Publishers Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Mols. of the title compound, C₂₈H₂₇ClN₄O₄·C₂H₆O, form a C(6) chain via an N-H...O H bond along the c axis by the operation of a c-glide plane, with N...O = 2.761(3) Å and N-H...O = 165°. The mols. are further linked by a weak C-H...O interaction, with C...O = 3.344(4) Å and C-H...O = 150°. Pendant H-bonded EtOH solvent mols. are attached to the chains by O-H...N H bonds, with O...N = 2.904(3) Å and O-H...N = 175°. Crystallog. data are given.

IT 382591-38-0P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and crystal structure of)

RN 382591-38-0 HCAPLUS

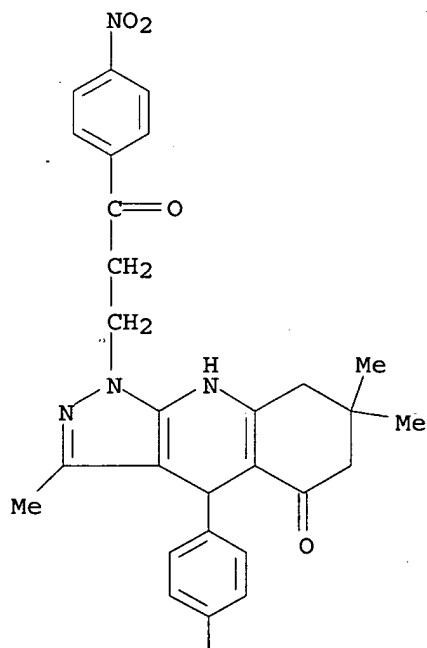
CN 5H-Pyrazolo[3,4-b]quinolin-5-one, 4-(4-chlorophenyl)-1,4,6,7,8,9-hexahydro-3,7,7-trimethyl-1-[3-(4-nitrophenyl)-3-oxopropyl]-, compd. with ethanol (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 382591-37-9

CMF C28 H27 Cl N4 O4

PAGE 1-A



PAGE 2-A

Cl

CM 2

CRN 64-17-5

CMF C2 H6 O

 $\text{H}_3\text{C}-\text{CH}_2-\text{OH}$

REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L36 ANSWER 3 OF 8 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2001:538846 HCAPLUS

DOCUMENT NUMBER: 135:331371

TITLE: Regioselective synthesis of 4,7,8,9-tetrahydro-2H-pyrazolo[3,4-b]quinolin-5(6H)-ones. Mechanism and structural analysis

AUTHOR(S): Quiroga, J.; Mejia, D.; Insuasty, B.; Abonia, R.; Nogueras, M.; Sanchez, A.; Cobo, J.; Low, J. N.

CORPORATE SOURCE: Departamento de Quimica, Grupo de Investigacion de Compuestos Heterociclicos, Universidad del Valle, Cali, 25360, Colombia

SOURCE: Tetrahedron (2001), 57(32), 6947-6953

CODEN: TETRAB; ISSN: 0040-4020

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 135:331371

AB Reactions of 5-amino-3-methyl-1H-pyrazole with dimedone and aldehydes afford regioselectively tricyclic linear 3,7,7-trimethyl-4,7,8,9-tetrahydro-2H-pyrazolo[3,4-b]quinolin-5(6H)-ones I (R = Ph, 3-pyridinyl, β -naphthalenyl, etc.) in good yields. Several aspects on this regioselective reaction, such as the reaction mechanism and structural studies of the predominant tautomeric form, are investigated.

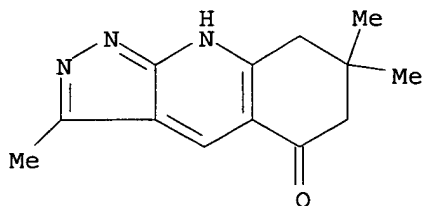
IT 370588-30-0P

RL: SPN (Synthetic preparation); PREP (Preparation)

(regioselective synthesis of pyrazoloquinolinones by cyclocondensation of aldehydes with aminomethylpyrazole and dimedone and mechanism)

RN 370588-30-0 HCAPLUS

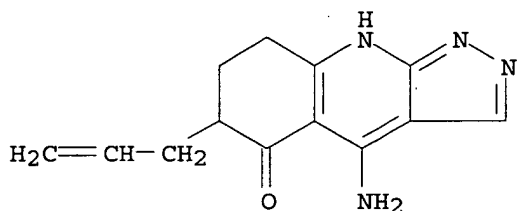
CN 5H-Pyrazolo[3,4-b]quinolin-5-one, 1,6,7,8-tetrahydro-3,7,7-trimethyl-(9CI) (CA INDEX NAME)



REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

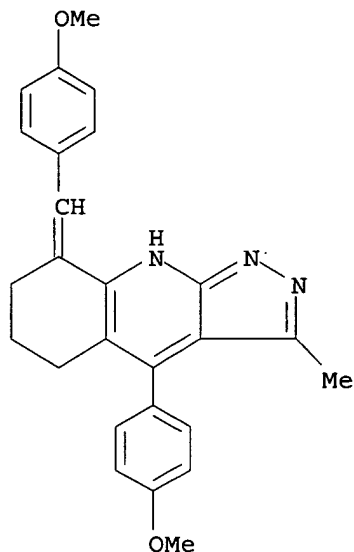
L36 ANSWER 4 OF 8 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1996:117818 HCAPLUS
 DOCUMENT NUMBER: 124:260921
 TITLE: Trimethylaluminum-promoted cyclization of cyanoenaminones. A versatile synthesis of substituted pyrazolopyridines
 AUTHOR(S): Campbell, James B.; Firor, Judy W.
 CORPORATE SOURCE: Medicinal Chem. Dep., Zeneca Pharmaceuticals, Wilmington, DE, 19897, USA
 SOURCE: Synthetic Communications (1996), 26(5), 981-90
 CODEN: SYNCAV; ISSN: 0039-7911
 PUBLISHER: Dekker
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 124:260921
 AB The readily available and inexpensive trimethylaluminum was used to effect the facile cyclization of cyanoenaminones to give the corresponding pyrazolopyridine derivs. Certain functional groups and sensitive side-chains, such as the 2-chloroethyl group, nitrile and alkyne, may be accommodated by the reaction.
 IT 99162-92-2P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation of pyrazolopyridines by trimethylaluminum-promoted cyclization of cyanoenaminones)
 RN 99162-92-2 HCAPLUS
 CN 5H-Pyrazolo[3,4-b]quinolin-5-one, 4-amino-1,6,7,8-tetrahydro-6-(2-propenyl)- (9CI) (CA INDEX NAME)

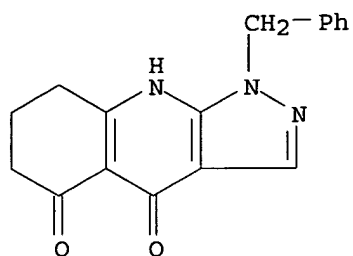


L36 ANSWER 5 OF 8 HCAPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 1994:605193 HCAPLUS
 DOCUMENT NUMBER: 121:205193
 TITLE: Reactions with 4-p-anisyl -8-p-anisylidene-1,2,5,6,7,8-hexahydro-2-oxo-3-quinolinecarbonitrile
 AUTHOR(S): El-Nagdy, S.; Hamad, M.M.; Mahmoud, M.R.; Said, S.A.; Habashy, M.M.
 CORPORATE SOURCE: Fac. Sci., Ain Shams Univ., Cairo, Egypt
 SOURCE: Egyptian Journal of Chemistry (1992), Volume Date 1991, 34(2), 157-64
 CODEN: EGJCA3; ISSN: 0367-0422
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 121:205193
 AB Reactions of the title compound (I) with Et bromoacetate, MeMgI, and POCl3 were studied. Thus, treatment of I with POCl3 gave II which reacted with hydrazine, phenylhydrazine, aniline, benzyl amine, p-toluidine, cyanoacetamide and 2-phenylethanoic hydrazide, in absolute ethanol to yield III (R=NH2, PhNH, Ph, PhCH2, p-MeC6H4, COCH2CN, PhCH2CONH).

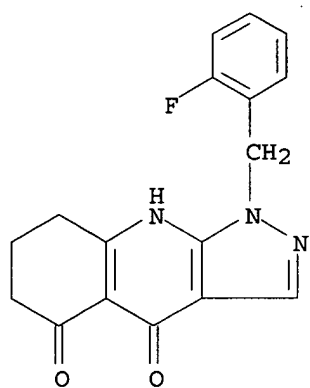
IT 157924-10-2P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 157924-10-2 HCAPLUS
 CN 1H-Pyrazolo[3,4-b]quinoline, 5,6,7,8-tetrahydro-4-(4-methoxyphenyl)-8-[(4-methoxyphenyl)methylene]-3-methyl- (9CI) (CA INDEX NAME)



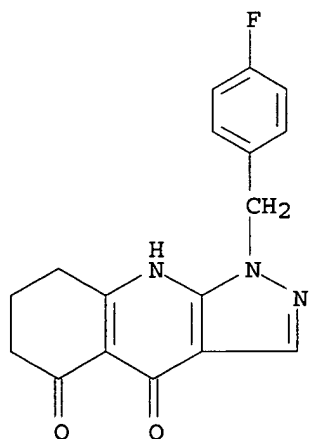
L36 ANSWER 6 OF 8 HCAPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 1991:656057 HCAPLUS
 DOCUMENT NUMBER: 115:256057
 TITLE: Synthesis of 7,8-dihydro-6H-pyrazolo[3,4-b]quinolin-5-ones and related derivatives
 AUTHOR(S): Gatta, Franco; Pomponi, Massimo; Marta, Maurizio
 CORPORATE SOURCE: Lab. Chim. Farm., Ist. Super. Sanita, Rome, 00161, Italy
 SOURCE: Journal of Heterocyclic Chemistry (1991), 28(5), 1301-7
 CODEN: JHTCAD; ISSN: 0022-152X
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB The synthesis of a new series of 4-amino-1-(unsubstituted and chloro or fluoro substituted benzyl)dihydropyrazoloquinolinones I (R = CH₂Ph, 2-, 4-FC₆H₄CH₂, 4-ClC₆H₄CH₂ or 2,4-Cl₂C₆H₃CH₂) and the corresponding diones II. from the corresponding benzylaminopyrazoles III (R₁ = CN, CO₂H, CO₂Et) is reported. The cyclocondensation of I or II with NaN₃ gave azepinones IV or isoxazoles V, resp.
 IT 137279-14-2P 137279-15-3P 137279-16-4P
 137279-17-5P 137279-18-6P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and cyclocondensation of, with sodium nitride)
 RN 137279-14-2 HCAPLUS
 CN 1H-Pyrazolo[3,4-b]quinoline-4,5(6H,9H)-dione, 7,8-dihydro-1-(phenylmethyl)- (9CI) (CA INDEX NAME)



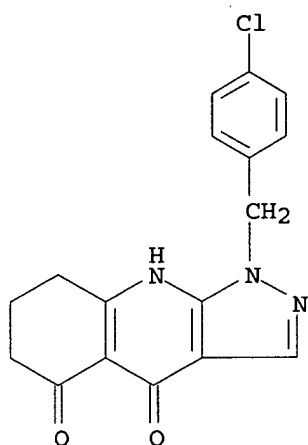
RN 137279-15-3 HCAPLUS
 CN 1H-Pyrazolo[3,4-b]quinoline-4,5(6H,9H)-dione, 1-[(2-fluorophenyl)methyl]-7,8-dihydro- (9CI) (CA INDEX NAME)



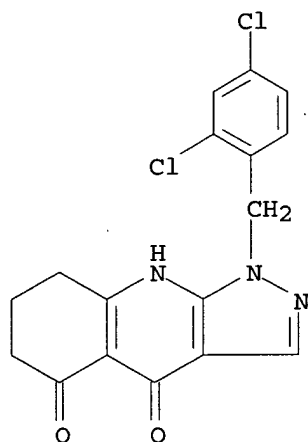
RN 137279-16-4 HCAPLUS
 CN 1H-Pyrazolo[3,4-b]quinoline-4,5(6H,9H)-dione, 1-[(4-fluorophenyl)methyl]-7,8-dihydro- (9CI) (CA INDEX NAME)



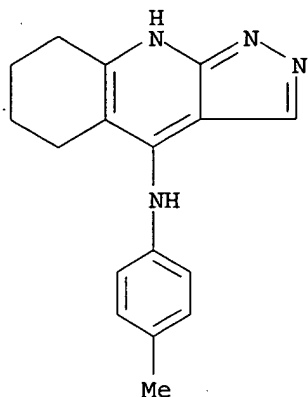
RN 137279-17-5 HCAPLUS
 CN 1H-Pyrazolo[3,4-b]quinoline-4,5(6H,9H)-dione, 1-[(4-chlorophenyl)methyl]-7,8-dihydro- (9CI) (CA INDEX NAME)



RN 137279-18-6 HCAPLUS
 CN 1H-Pyrazolo[3,4-b]quinoline-4,5(6H,9H)-dione, 1-[(2,4-dichlorophenyl)methyl]-7,8-dihydro- (9CI) (CA INDEX NAME)

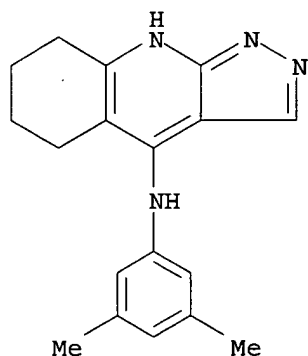


L36 ANSWER 7 OF 8 HCAPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 1986:608800 HCAPLUS
 DOCUMENT NUMBER: 105:208800
 TITLE: Phosphorus pentoxide in organic synthesis. XXIX. Synthesis of 4-arylamino-5,6,7,8-tetrahydro-1H-pyrazolo[3,4-b]quinolines and the corresponding N-Mannich bases
 AUTHOR(S): Nielsen, Soren V.; Pedersen, Erik B.
 CORPORATE SOURCE: Dep. Chem., Odense Univ., Odense, DK-5230, Den.
 SOURCE: Liebigs Annalen der Chemie (1986), (10), 1728-35
 CODEN: LACHDL; ISSN: 0170-2041
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 105:208800
 AB Title pyrazoloquinolines I (R = H, R1 = arylamino) (II) were prepared (8-52%



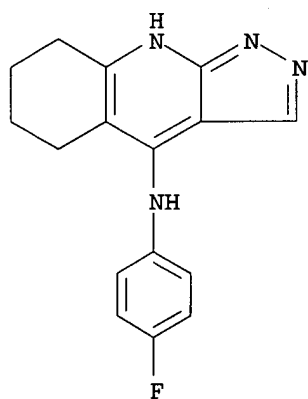
RN 103259-38-7 HCAPLUS

CN 1H-Pyrazolo[3,4-b]quinolin-4-amine, N-(3,5-dimethylphenyl)-5,6,7,8-tetrahydro- (9CI) (CA INDEX NAME)



RN 103259-39-8 HCAPLUS

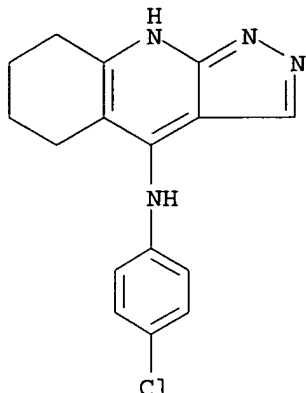
CN 1H-Pyrazolo[3,4-b]quinolin-4-amine, N-(4-fluorophenyl)-5,6,7,8-tetrahydro- (9CI) (CA INDEX NAME)



RN 103259-40-1 HCAPLUS

CN 1H-Pyrazolo[3,4-b]quinolin-4-amine, N-(4-chlorophenyl)-5,6,7,8-tetrahydro-

(9CI) (CA INDEX NAME)



L36 ANSWER 8 OF 8 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1985:615280 HCAPLUS

DOCUMENT NUMBER: 103:215280

TITLE: Pyrazolopyridine cycloalkanone derivatives

INVENTOR(S): Campbell, James Boniface, Jr.; Bare, Thomas Michael

PATENT ASSIGNEE(S): ICI Americas, Inc., USA

SOURCE: Eur. Pat. Appl., 115 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 141608	A2	19850515	EP 1984-307272	19841023
EP 141608	A3	19880302		
R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE				
US 4546104	A	19851008	US 1984-659615	19841011
ZA 8408352	A	19850626	ZA 1984-8352	19841025
FI 8404296	A	19850505	FI 1984-4296	19841101
DK 8405229	A	19850505	DK 1984-5229	19841102
NO 8404376	A	19850506	NO 1984-4376	19841102
AU 8434949	A1	19850509	AU 1984-34949	19841102
HU 35679	O	19850729	HU 1984-4064	19841102
ES 537338	A1	19860101	ES 1984-537338	19841102
JP 60115581	A2	19850622	JP 1984-231445	19841105

PRIORITY APPLN. INFO.: GB 1983-29531 19831104

AB The title compds. [I: R, R2 = H, (substituted) alkyl; R1 = H, alkyl; R3, R4 = H, (substituted) alkyl, CR3R4 = ring; R5, R6 = H, alkyl, alkenyl; X = bond, alkylene] were prepared. Thus, heating a mixture 1.65 g pyrazole derivative

II, 20 mL xylenes, and 12 g ZnCl₂ for 2 h gave 0.68 g I (R = pentyl, R1-R6 = H, X = CH₂). All I exhibited anxiolytic activity in rats.

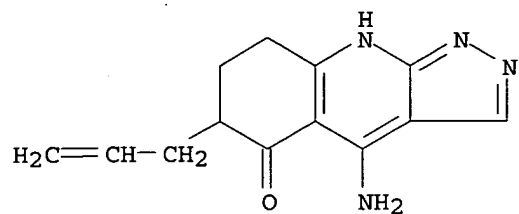
IT 99162-92-2P 99162-95-5P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and alkylation and anxiolytic activity of)

RN 99162-92-2 HCAPLUS

CN 5H-Pyrazolo[3,4-b]quinolin-5-one, 4-amino-1,6,7,8-tetrahydro-6-(2-

propenyl)- (9CI) (CA INDEX NAME)



RN 99162-95-5 HCAPLUS

CN 5H-Pyrazolo[3,4-b]quinolin-5-one, 4-amino-6-(3,3-dichloro-2-propenyl)-
1,6,7,8-tetrahydro- (9CI) (CA INDEX NAME)

